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Coarse-graining dislocation dynamics with length distributions

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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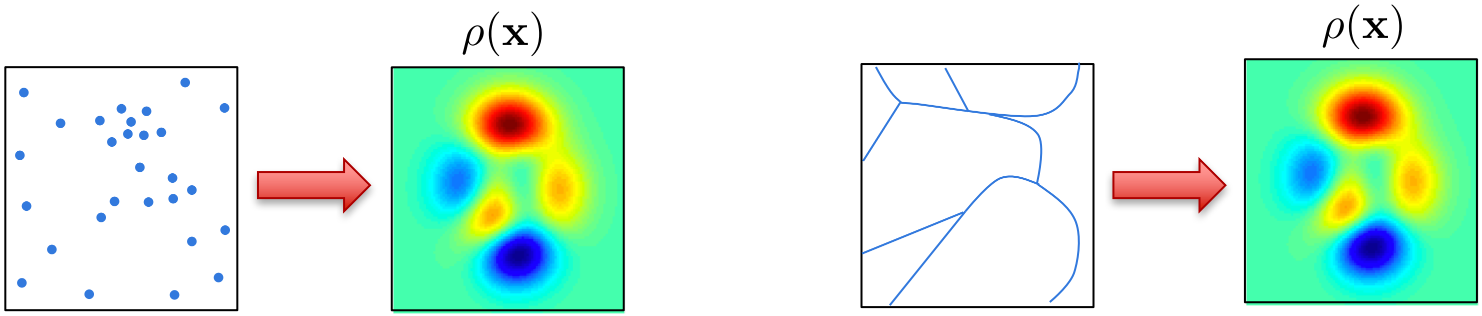
Down with density fields

- Homogenization via density fields is simplest approach to coarse-graining

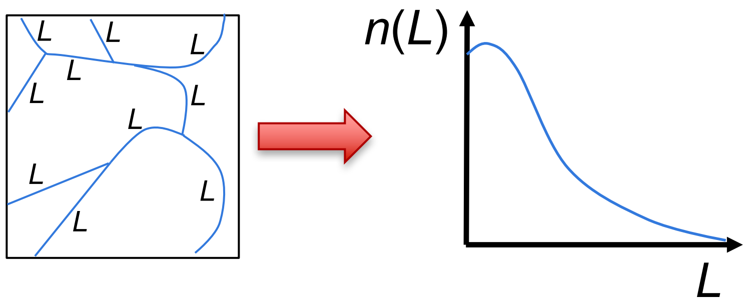


- Major drawbacks for dislocation structures:
  - No concept of topology/connectivity between lines
  - Hard to relate "unit processes" to governing equations
    - Bowing out, junction formation, cross-slip…

$$\frac{\partial \rho(t, \mathbf{x})}{\partial t} = \ldots$$

Long live length distributions

- Length distributions contain a lot more information!



n(*L*)*dL* = number density per unit volume of links of length *L*

$$\rho = \int_0^\infty L n(L) dL$$

$$N = \int_0^\infty n(L) dL$$

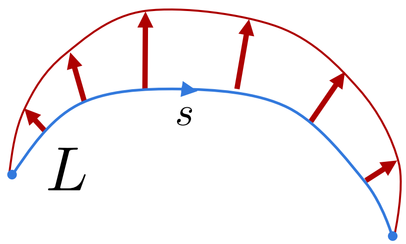
$$\frac{\partial n(t, L, \mathbf{x})}{\partial t} = \ldots$$

- Idea originally proposed by Lagneborg and Forsen (1973)
  - Ostrom and Lagneborg (1976), Ardell et al. (1984, 1986, 1989, 2002), Nix et al. (1974, 1979)
  - But that's about it…. Why?

$n(L)$ governing equations

$$\frac{\partial n(t,L)}{\partial t} = \dot{n}_{\mathrm{drift}}(L) + \dot{n}_{\mathrm{coll}}(L) + \ldots$$

$v(s) \rightarrow \dot{L}(L),\ \dot{A}(L)$



"Drift" term accounts for elongation of links

"Collision" term accounts for forest collisions and junction formation

$$\dot{n}_{\mathrm{drift}}(L) = -\frac{\partial}{\partial t}\left(n(L)\cdot\dot{L}(L)\right)$$

Elongation rate

$$\dot{n}_{\mathrm{coll}} = \dot{n}_{\mathrm{coll}}(\dot{A}(L))$$

Area sweep rate

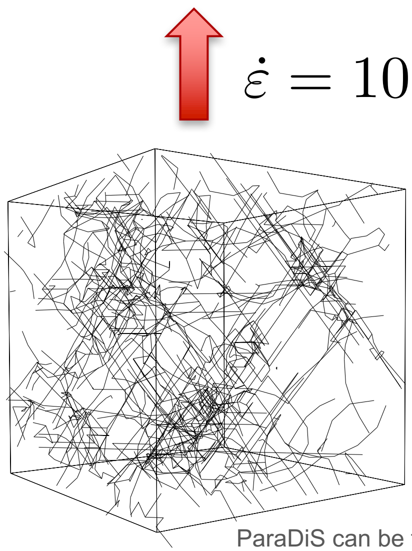
- How do we determine $\dot{L}(L),\ \dot{A}(L)$?
  - Density-based theories need constitutive *parameters*, here we need constitutive *laws*!

Discrete Dislocation Dynamics

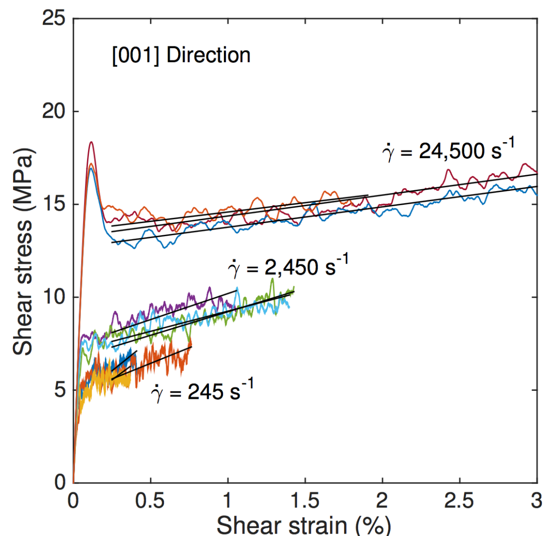
- DDD provides an elegant tool for determining link constitutive laws
  - Constitutive *laws* easier to determine than constitutive *parameters*

[001]

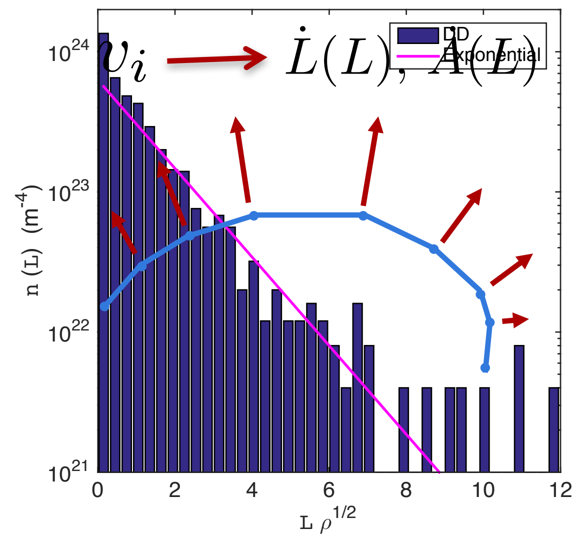
$\dot{\varepsilon} = 1000 \text{ s}^{-1}$



ParaDiS can be freely downloaded at
http://paradis.stanford.edu



Exponentially distributed!
Why?

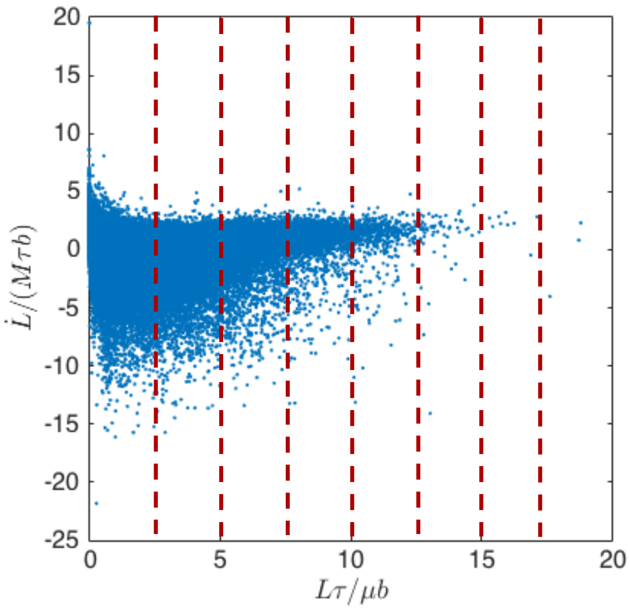


New subcycling-based time integrator gives 100x speedup
Sills et al. Modell. Simul. Mater. Sci. Eng. 24 (2016)

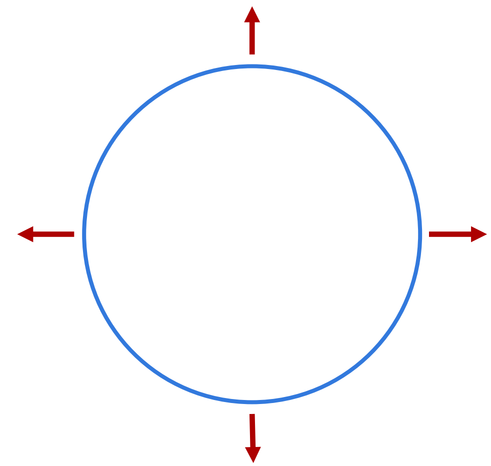
Coarse-graining with DDD

- 7.6 million data points from 6 independent DDD simulations

Raw Data



$$\dot{L}/\tau, \dot{A} \propto L\tau$$



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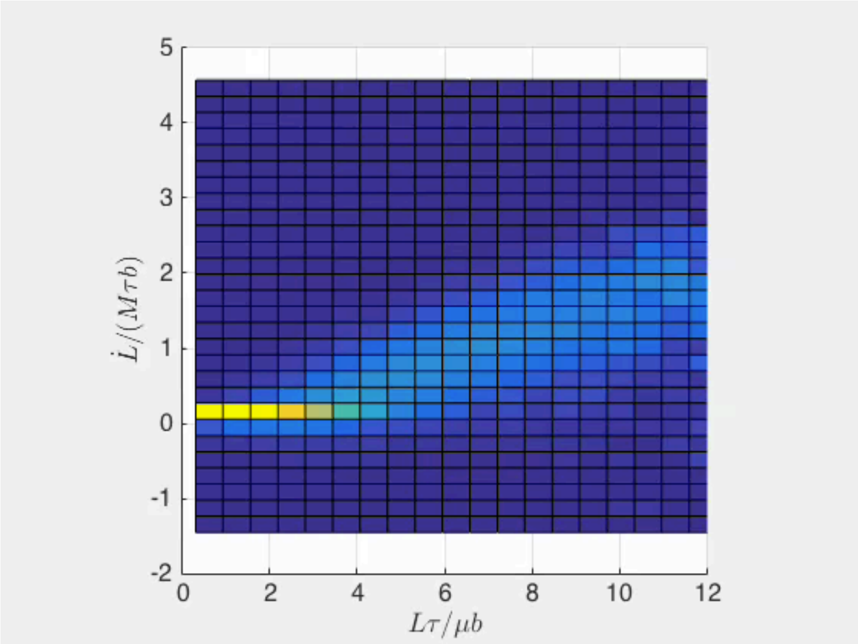
Normalized Histogram



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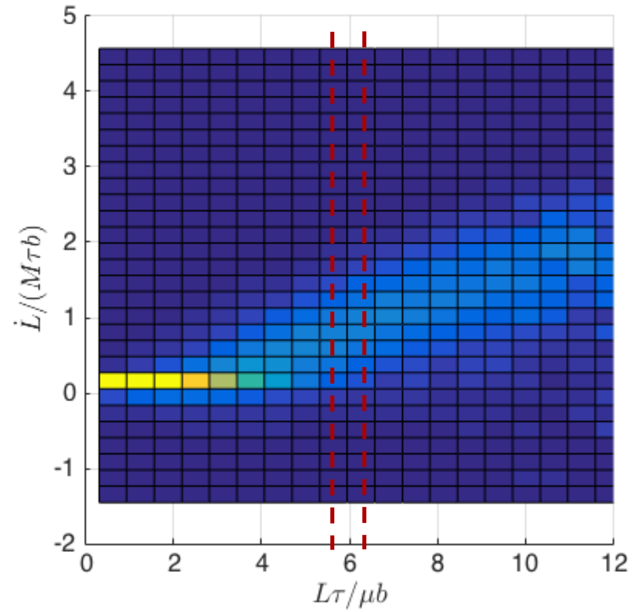

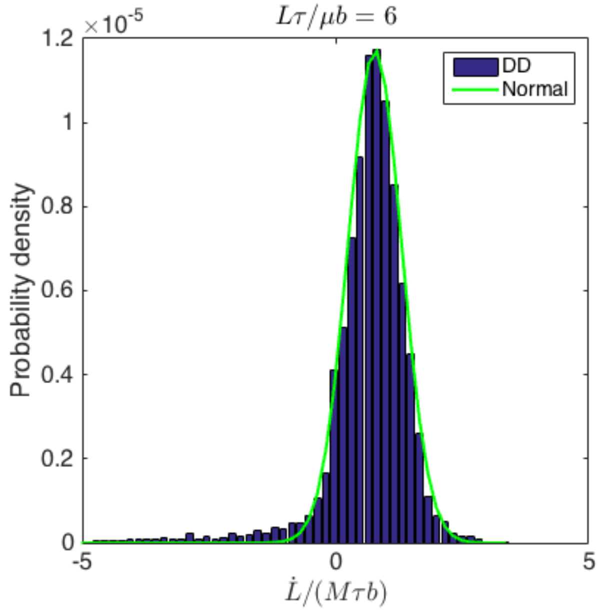

Coarse-graining with DDD

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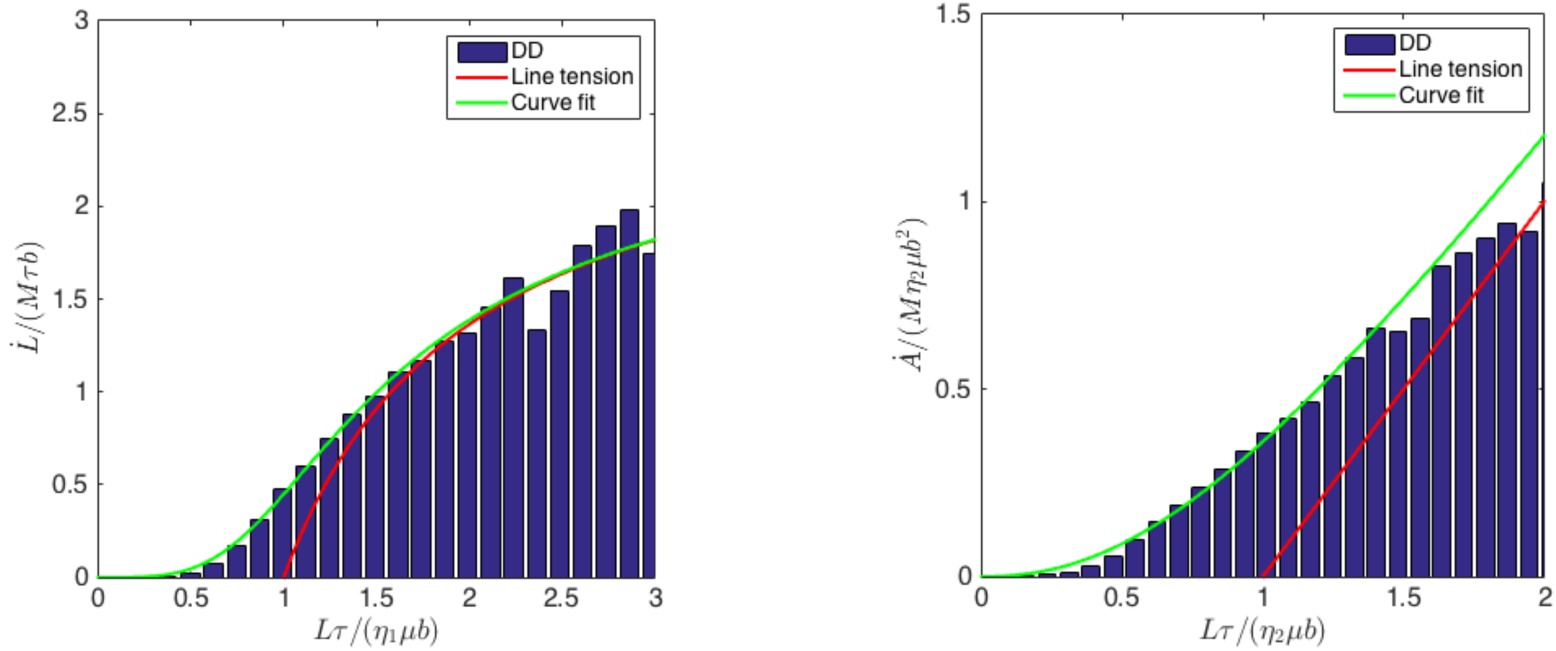
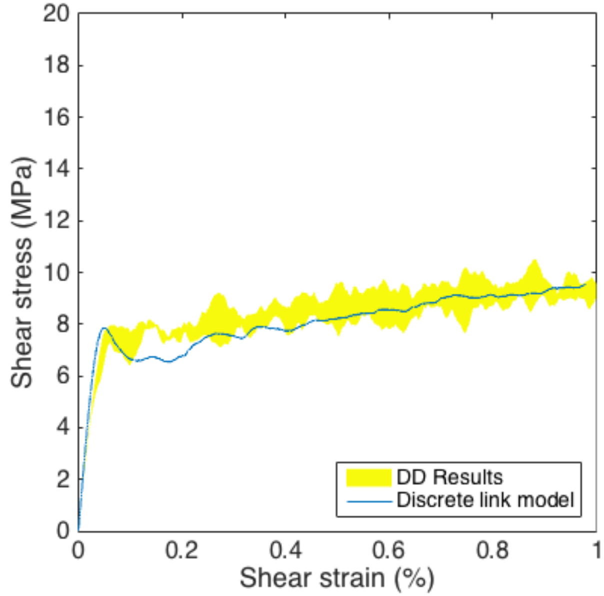
Median values in each bin

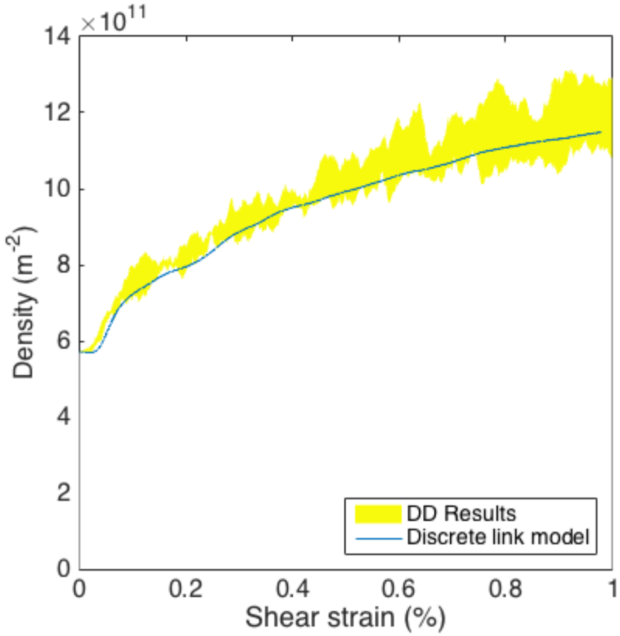


Preliminary results

- "Discrete link model" - Array of independent links
- At each time step:
  - Bow out
  - Sweep area (produce plastic strain)
  - Collide with each other randomly (form stable junctions)

Preliminary results





- Currently unable to extract all junction formation info
- Need to add an ad hoc annihilation term
  - Still under investigation

Preliminary results

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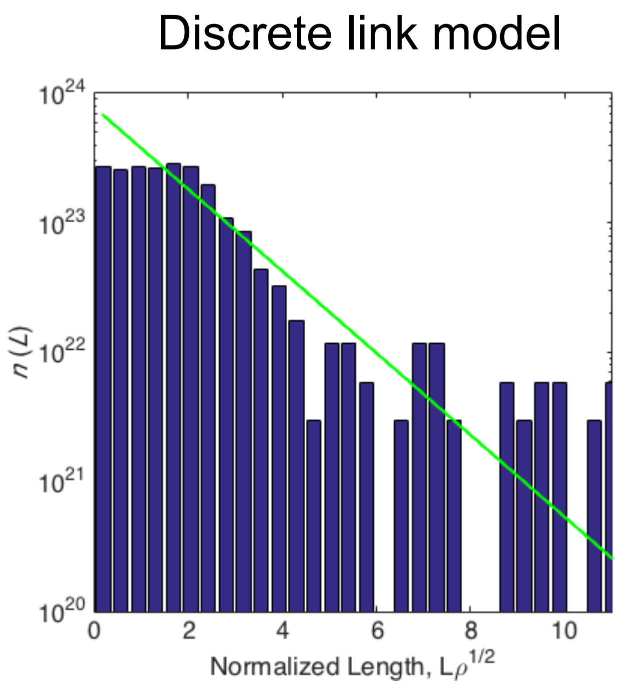

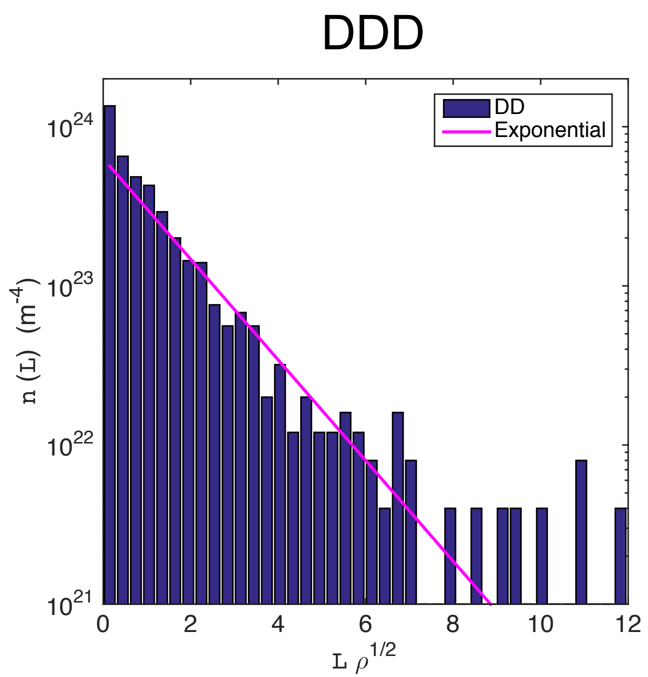

- Currently unable to extract all junction formation info
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Summary

- Length-distribution-based model provides richer description of dislocation microstructures
- Able to extract link constitutive laws directly from DDD simulations
- Initial results provide hope that coarse-graining based on length distributions describes physics of dislocation ensembles