The Thermal Field Dislocation Mechanics (T-FDM) model

Upadhyay, M. V., On the thermo-mechanical theory of field dislocations in transient heterogeneous temperature fields, *Journal of the Mechanics and Physics of Solids,* 105 (2020) 104150

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- Development
    - The isothermal and adiabatic FDM model
    - Heat conduction
    - The new T-FDM model
- Model assumptions and impact on AM modelling

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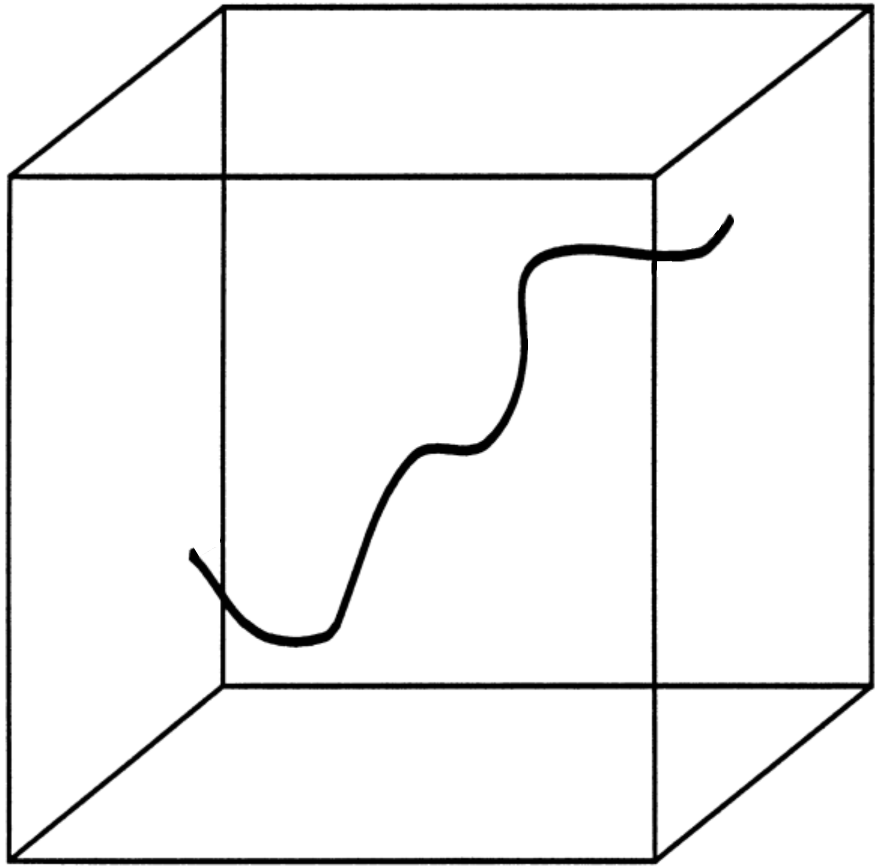
Representing dislocations in a continuum



Adapted from *Arsenlis, Parks, Acta Mat. (1999)*

- <u>Discrete representation</u>

  A line (singular) defect

  Michell 1899, Timpe 1905, Weingarten 1901, Volterra 1907, Love 1944, Nabarro 1967, Hirth & Lothe 1982

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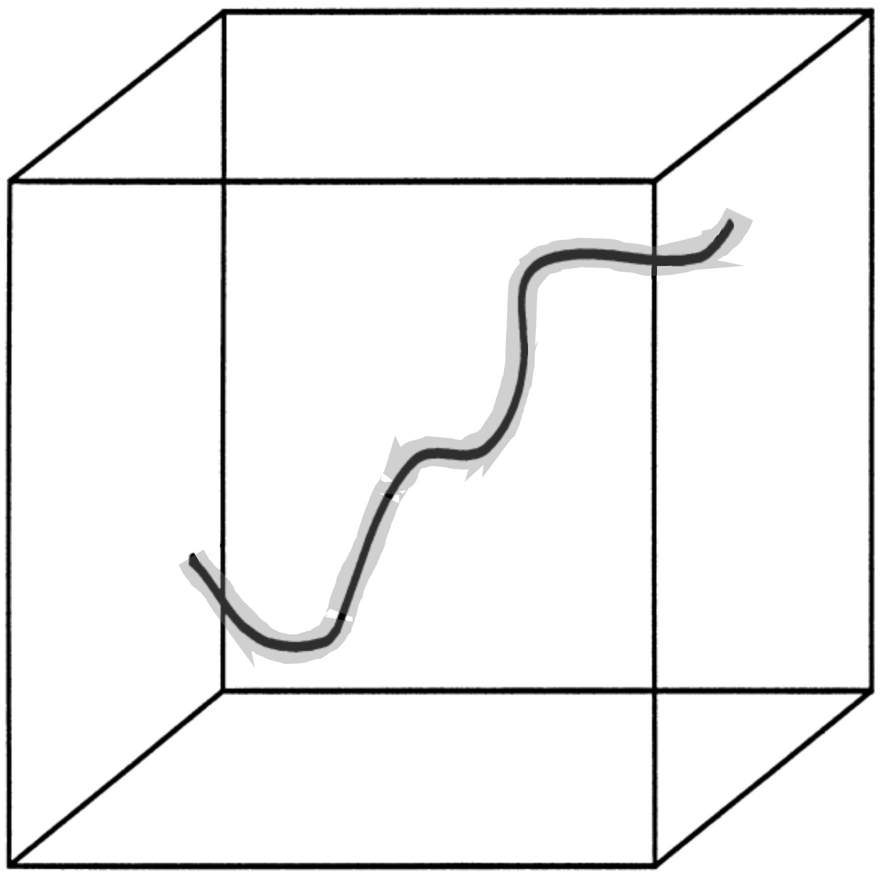

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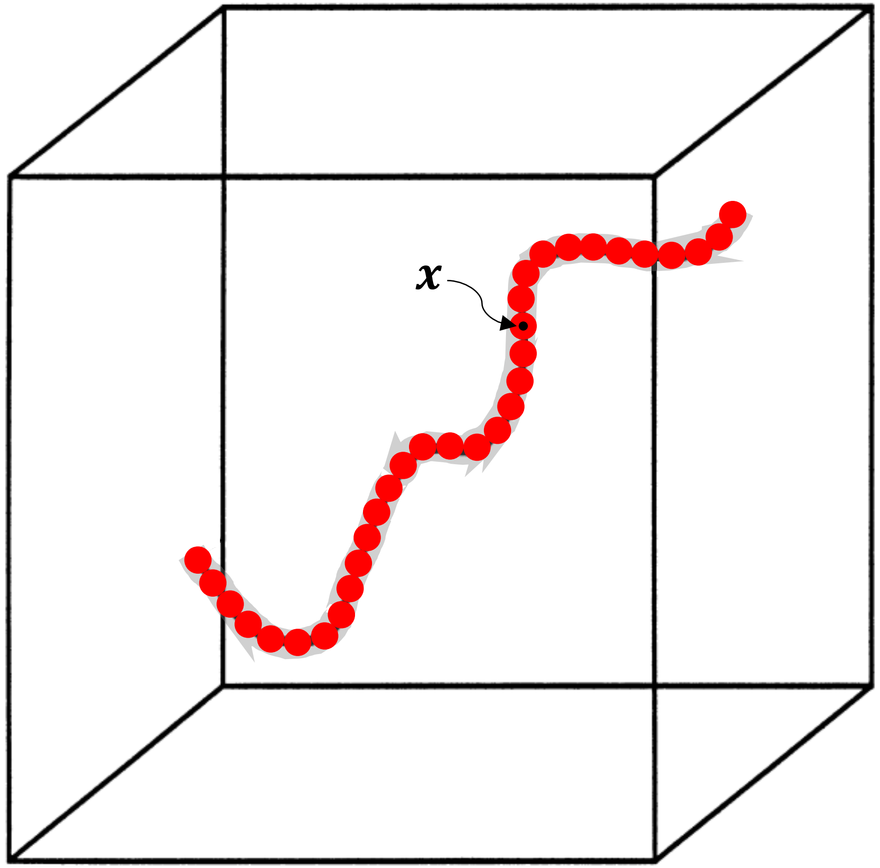
Continuous representation

Smearing out the line over a finite volume V

Representing dislocations in a continuum



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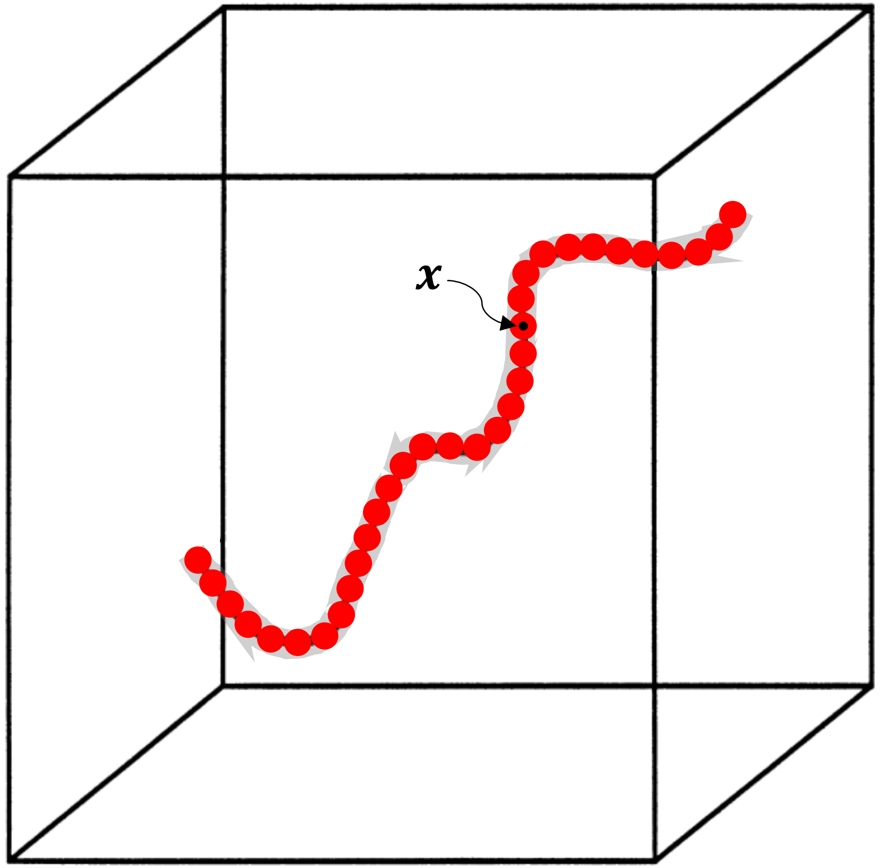
Smearing out the line over a finite volume V

Represent via a finite non-zero polar density $\bar{\bar{\boldsymbol{\alpha}}}$

$$\bar{\bar{\boldsymbol{\alpha}}}(\bar{\boldsymbol{x}}) = \frac{1}{V_{sphere}} f(dislocation\ character)$$

Nye 1953, Kroener 1958, Mura 1963, Willis 1967, Kosevich 1979, Kröner 1981, Acharya group 2001 - 2020

Representing dislocations in a continuum



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Limit condition

Continuous representation

Smearing out the line over a finite volume V

⬇

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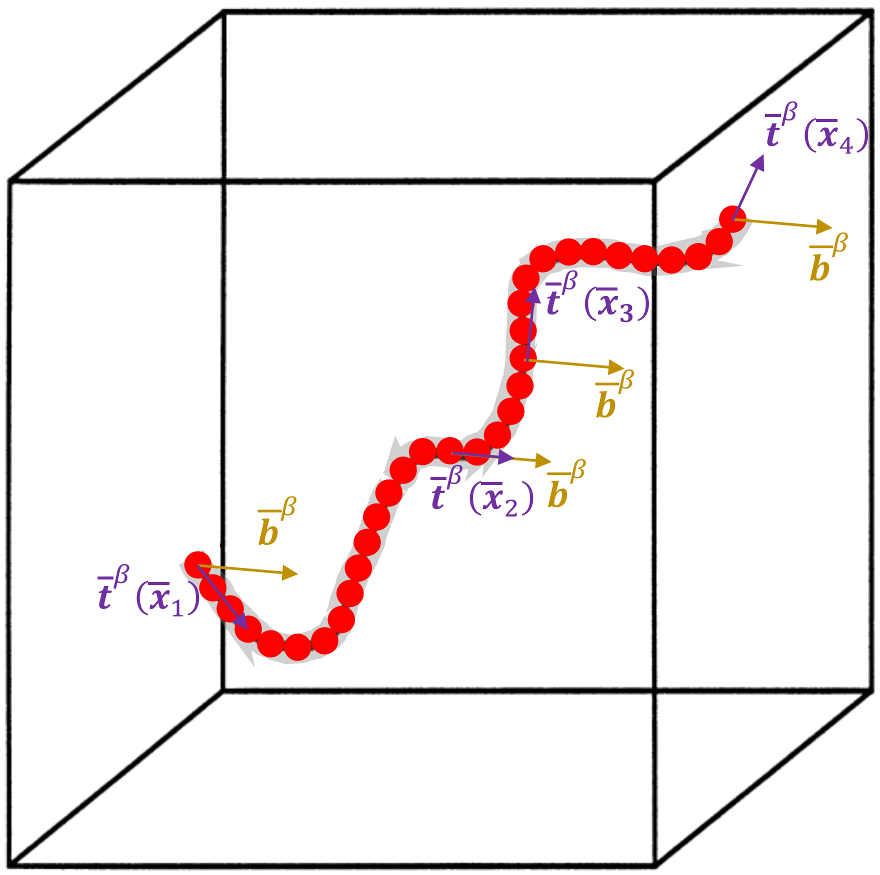
Theory of continuously represented dislocations: characterization



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<u>A single dislocation on a slip system $\boldsymbol{\beta}$</u>

Characterized via Burgers vector $\bar{\boldsymbol{b}}^{\beta}$ and local unit tangent to dislocation line $\hat{\boldsymbol{t}}^{\beta}(\bar{\boldsymbol{x}})$

$$\bar{\bar{\boldsymbol{\alpha}}}^{\beta}(\bar{\boldsymbol{x}}) = \frac{1}{V_{sphere}} \int_L \bar{\boldsymbol{b}}^{\beta} \otimes \hat{\boldsymbol{t}}^{\beta}(\bar{\boldsymbol{x}}) dL$$

https://www.manas-upadhyay.com

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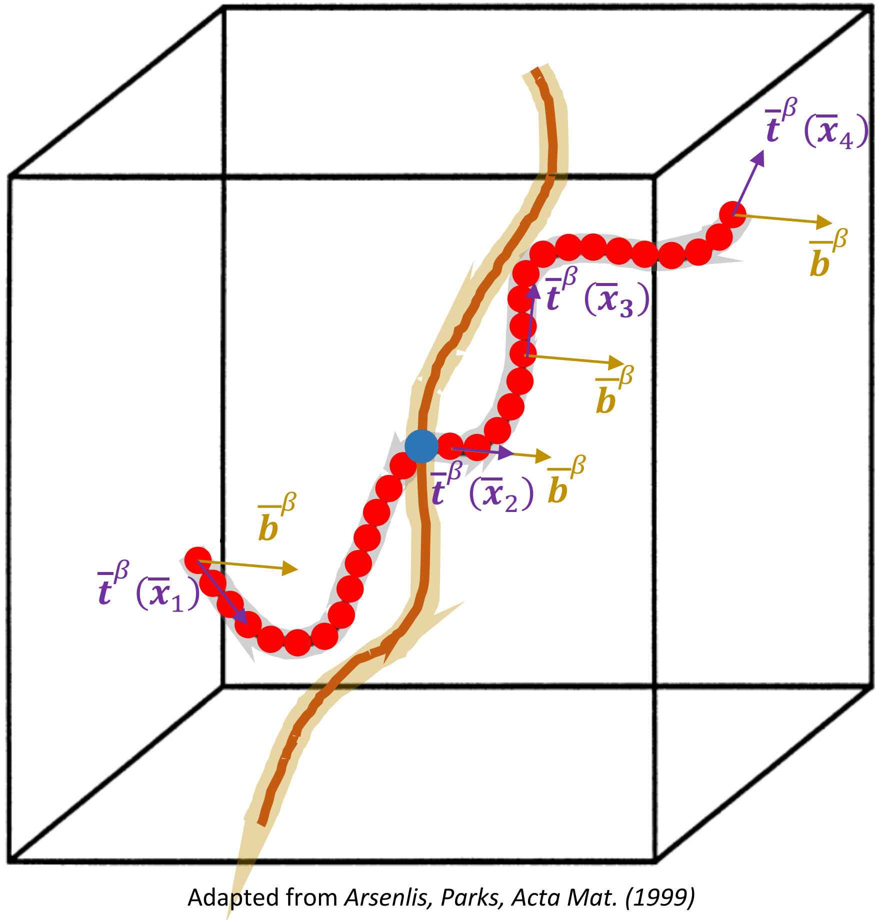

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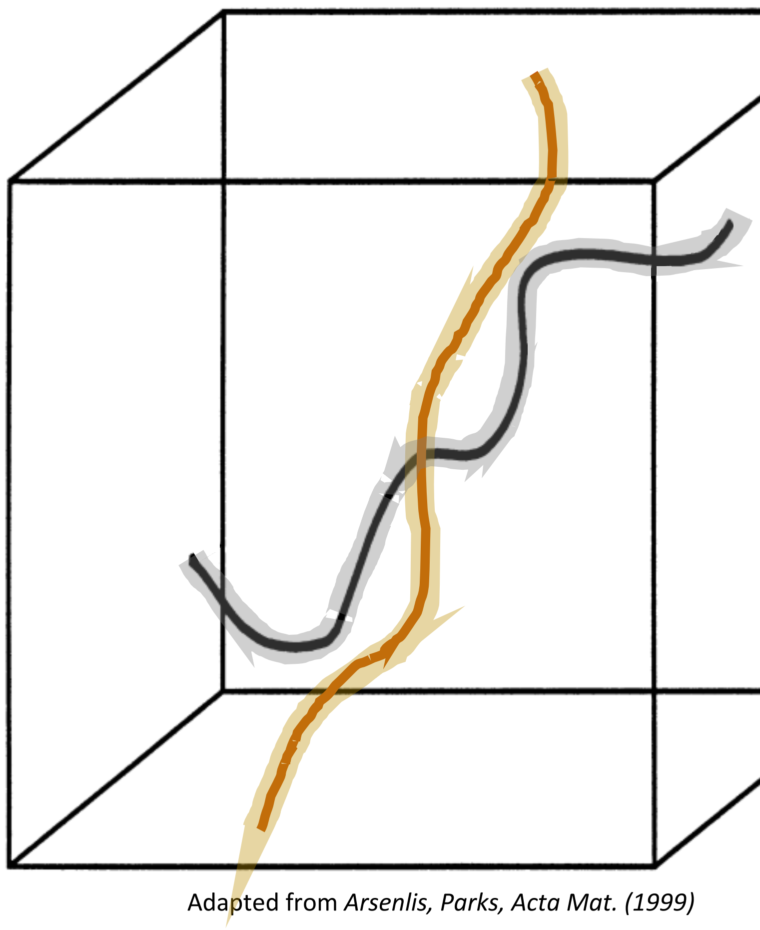
Multiple dislocations on different slip systems

$$\bar{\bar{\boldsymbol{\alpha}}}(\bar{\boldsymbol{x}}) = \sum_{\beta} \bar{\bar{\boldsymbol{\alpha}}}^{\beta}(\bar{\boldsymbol{x}}) = \frac{1}{V_{sphere}} \int_L \sum_{\beta} \bar{\boldsymbol{b}}^{\beta}(\bar{\boldsymbol{x}}) \otimes \hat{\boldsymbol{t}}^{\beta}(\bar{\boldsymbol{x}})\, dL$$

Nye’s polar dislocation density tensor (Nye 1953)

Continuity condition: $\mathbf{div}\, \bar{\bar{\boldsymbol{\alpha}}} = \mathbf{0}$

Theory of continuously represented dislocations: deformation fields



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Assume simply connected domain

Total displacement $\overline{\boldsymbol{u}}$ continuous everywhere => $[\![\overline{\boldsymbol{u}}]\!] = \mathbf{0}$

Total distortion: $\overline{\overline{\boldsymbol{U}}}^{\parallel} = \mathbf{grad}\,\overline{\boldsymbol{u}} = \nabla\overline{\boldsymbol{u}}$ (“‖” => compatible)

$$\mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{\parallel} = \mathbf{0}$$

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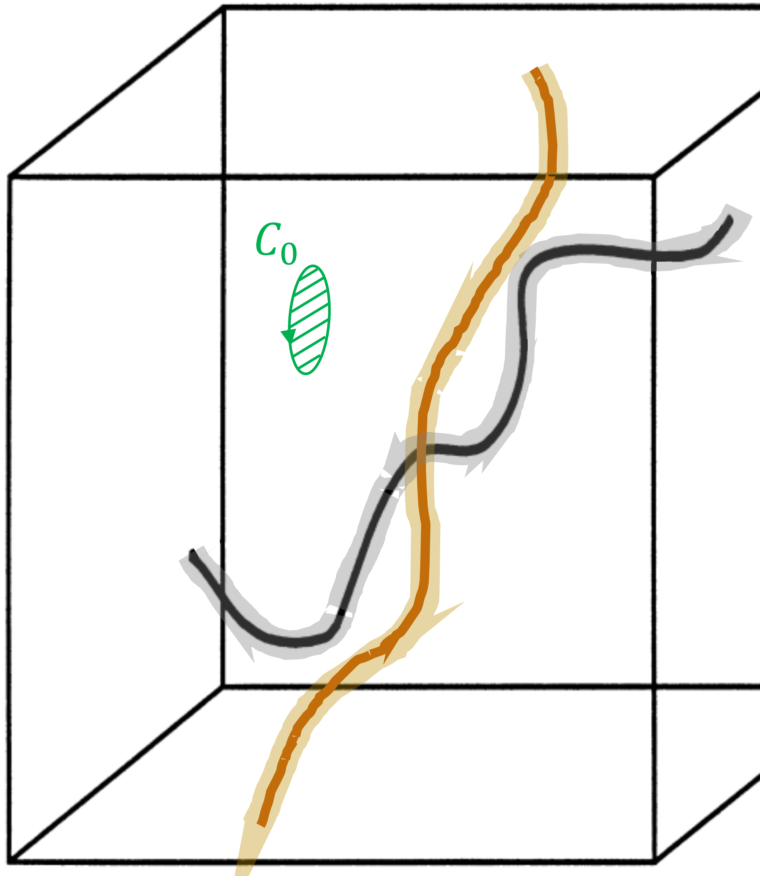

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Locations without dislocations (Circuit C_0)

$$[\![\overline{\boldsymbol{u}}^{e}]\!] = \mathbf{0} \quad \Rightarrow \quad \overline{\overline{\boldsymbol{U}}}^{e\parallel} = \mathbf{grad}\,\overline{\boldsymbol{u}}^{e} \quad \Rightarrow \quad \mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{e\parallel} = \mathbf{0}$$

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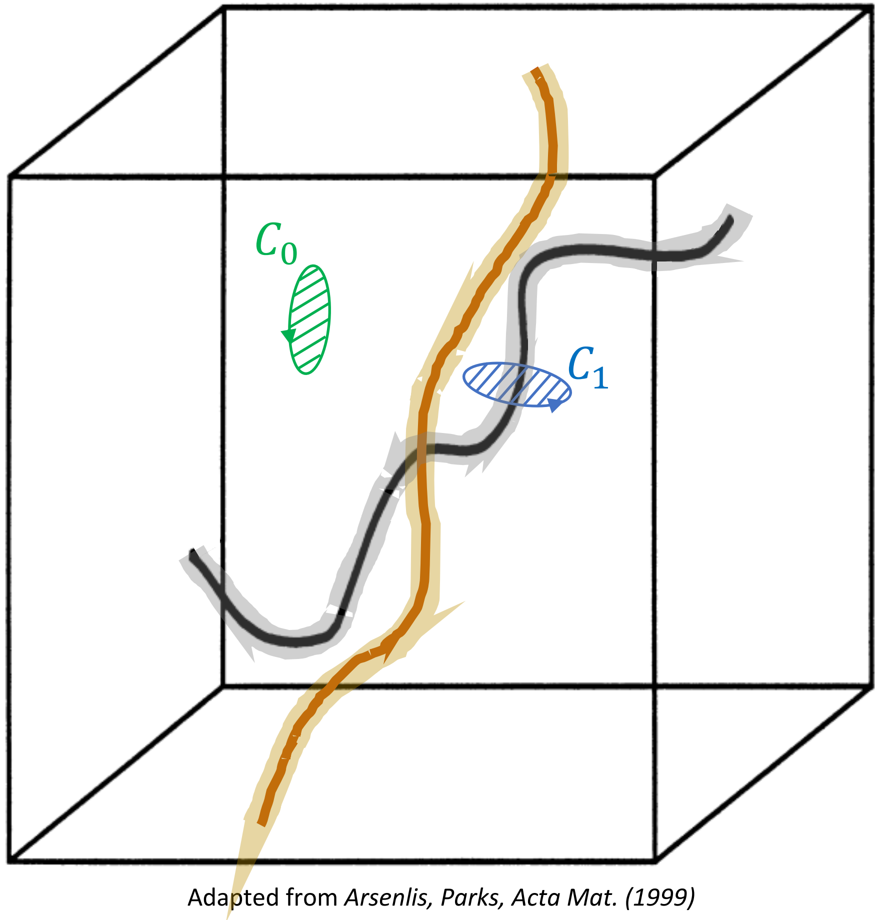

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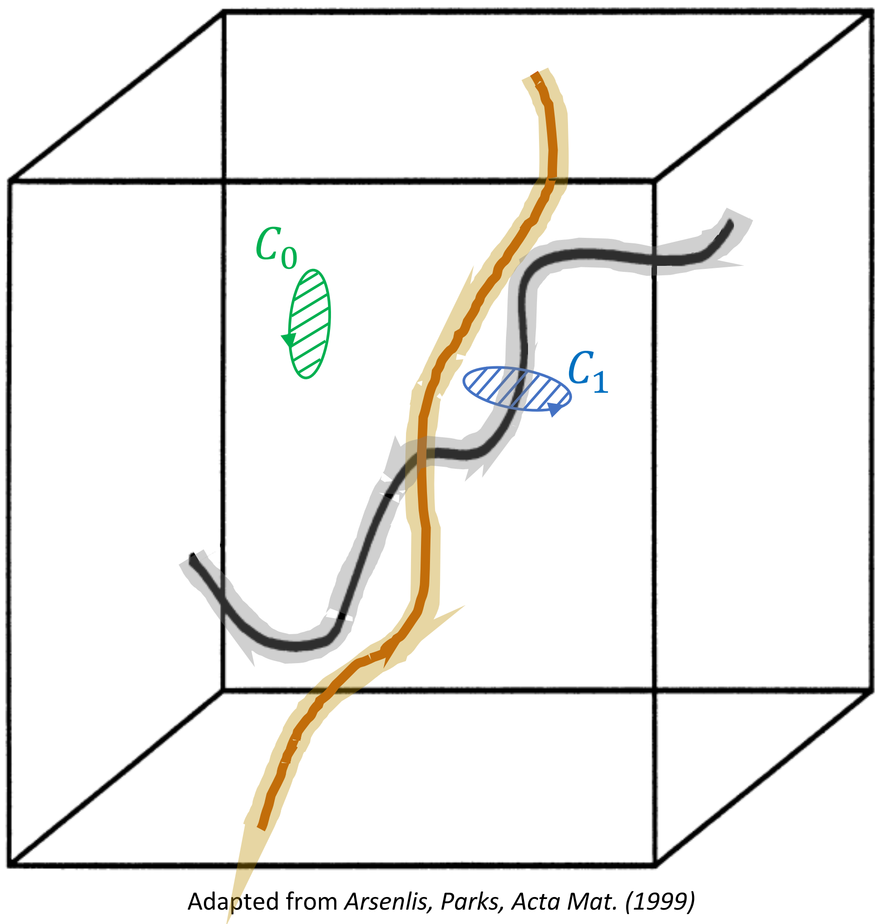
Locations with dislocations (Circuit C_1)

$$\overline{\boldsymbol{b}}^{\beta} = [\![\overline{\boldsymbol{u}}^{e,\beta}]\!] = \int_{C_1} \overline{\overline{\boldsymbol{U}}}^{e,\beta} \cdot \overline{\boldsymbol{dL}} = \int_{S_1} \left(\mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{e,\beta}\right) \cdot \overline{\boldsymbol{n}}_1\, dS \neq \mathbf{0}$$

Theory of continuously represented dislocations: deformation fields



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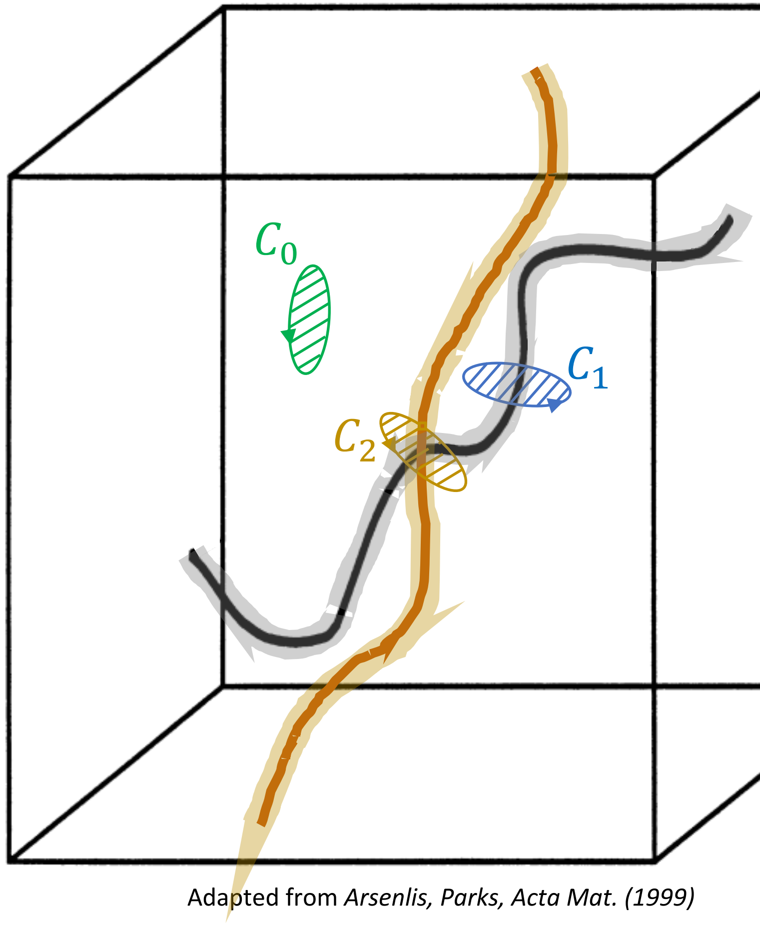
$$\mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{e,\beta} \neq \mathbf{0} \Rightarrow \overline{\overline{\boldsymbol{U}}}^{e,\beta} \neq \overline{\overline{\boldsymbol{U}}}^{e,\beta\parallel}$$

Theory of continuously represented dislocations: deformation fields



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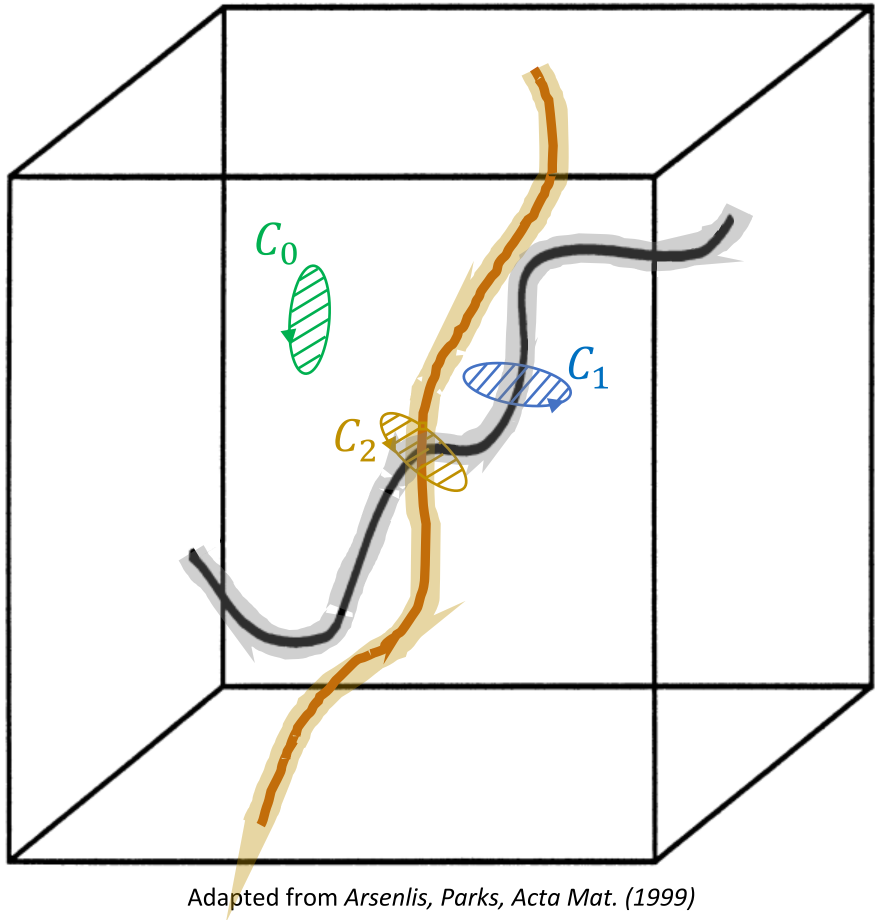
Locations with multiple dislocations (Circuit C_2)

$$\overline{\boldsymbol{b}} = [\![\overline{\boldsymbol{u}}^e]\!]^{\beta_1} + [\![\overline{\boldsymbol{u}}^e]\!]^{\beta_2} = \int_{C_3} \overline{\overline{\boldsymbol{U}}}^e \cdot \overline{\boldsymbol{dL}} = \int_{S_3} \underbrace{\mathbf{curl}\, \overline{\overline{\boldsymbol{U}}}^e}_{\overline{\overline{\boldsymbol{\alpha}}}} \cdot \overline{\boldsymbol{n}}_3 \, dS \neq 0$$

Theory of continuously represented dislocations: deformation fields



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Now,

$$\bar{\bar{\boldsymbol{\alpha}}} = \sum_{\beta} \bar{\bar{\boldsymbol{\alpha}}}^{\beta} \Rightarrow \mathbf{curl}\, \bar{\bar{\boldsymbol{U}}}^e = \sum_{\beta} \mathbf{curl}\, \bar{\bar{\boldsymbol{U}}}^{e,\beta}$$

But

$$\bar{\bar{\boldsymbol{U}}}^e \neq \sum_{\beta} \bar{\bar{\boldsymbol{U}}}^{e\beta}$$

Also

$$\boxed{\bar{\bar{\boldsymbol{U}}}^e \neq \bar{\bar{\boldsymbol{U}}}^{e\parallel}}$$

Stokes-Helmholtz type decomposition of $\overline{\overline{\boldsymbol{U}}}^e$

Acharya and Roy JMPS 54 (2006) 1687 – 1710

Additive decomposition of $\overline{\overline{\boldsymbol{U}}}^e$ into compatible $\overline{\overline{\boldsymbol{U}}}^{e\parallel}$ and incompatible $\overline{\overline{\boldsymbol{U}}}^{e\perp}$

$$\overline{\overline{\boldsymbol{U}}}^e = \overline{\overline{\boldsymbol{U}}}^{e\parallel} + \overline{\overline{\boldsymbol{U}}}^{e\perp} \text{ in } \Omega$$

Stokes-Helmholtz type decomposition of $\overline{\overline{\boldsymbol{U}}}^e$

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Unique additive decomposition of $\bar{\bar{\boldsymbol{U}}}^e$ into compatible $\bar{\bar{\boldsymbol{U}}}^{e\parallel}$ and incompatible $\bar{\bar{\boldsymbol{U}}}^{e\perp}$

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$$\textbf{div}\,\bar{\bar{\boldsymbol{U}}}^{e\perp} = \boldsymbol{0} \text{ in } \Omega$$

$$\bar{\bar{\boldsymbol{U}}}^{e\perp} \cdot \bar{\boldsymbol{n}} = \boldsymbol{0} \text{ on } \partial\Omega$$

Stokes-Helmholtz type decomposition of $\overline{\overline{\boldsymbol{U}}}^{e}$

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<u>**Unique**</u> additive decomposition of $\overline{\overline{\boldsymbol{U}}}^{e}$ into compatible $\overline{\overline{\boldsymbol{U}}}^{e\parallel}$ and incompatible $\overline{\overline{\boldsymbol{U}}}^{e\perp}$

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$$\mathbf{div}\,\overline{\overline{\boldsymbol{U}}}^{e\perp} = \mathbf{0} \text{ in } \Omega$$

$$\overline{\overline{\boldsymbol{U}}}^{e\perp} \cdot \overline{\boldsymbol{n}} = \mathbf{0} \text{ on } \partial\Omega$$

$$\Rightarrow \overline{\overline{\boldsymbol{\alpha}}} = \mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{e} = \mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{e\perp} \neq \mathbf{0}$$

Elasto-static theory of dislocation fields

Question: Given $\overline{\overline{\boldsymbol{\alpha}}}^{\beta}$ (typically from experiments), how to obtain $\overline{\overline{\boldsymbol{U}}}^{e} = \overline{\overline{\boldsymbol{U}}}^{e\parallel} + \overline{\overline{\boldsymbol{U}}}^{e\perp}$?

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Answer:

1) For $\overline{\overline{\boldsymbol{U}}}^{e\perp}$: approach similar to the Helmholtz identity ($\mathbf{curl}\ \mathbf{curl}\ \overline{\overline{\boldsymbol{\chi}}} = \mathbf{grad}\ \mathbf{div}\ \overline{\overline{\boldsymbol{\chi}}} - \Delta\overline{\overline{\boldsymbol{\chi}}}$)

$\overline{\overline{\boldsymbol{\alpha}}} = \mathbf{curl}\ \overline{\overline{\boldsymbol{U}}}^{e\perp}$ and $\mathbf{div}\ \overline{\overline{\boldsymbol{U}}}^{e\perp} = \mathbf{0}$ gives $\Delta\overline{\overline{\boldsymbol{U}}}^{e\perp} = -\mathbf{curl}\ \overline{\overline{\boldsymbol{\alpha}}}$ (Acharya Roy JMPS 2006)

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2) For $\overline{\overline{\boldsymbol{U}}}^{e\parallel}$: mechanical equilibrium and elastic law

Mechanical (static) equilibrium: $\mathbf{div}\ \overline{\overline{\boldsymbol{\sigma}}} = \mathbf{0}$

Elastic constitutive law: $\overline{\overline{\boldsymbol{\sigma}}} = \overline{\overline{\overline{\overline{\boldsymbol{c}}}}} : \overline{\overline{\boldsymbol{\varepsilon}}}^{e} = \overline{\overline{\overline{\overline{\boldsymbol{c}}}}} : \overline{\overline{\boldsymbol{U}}}^{e}$

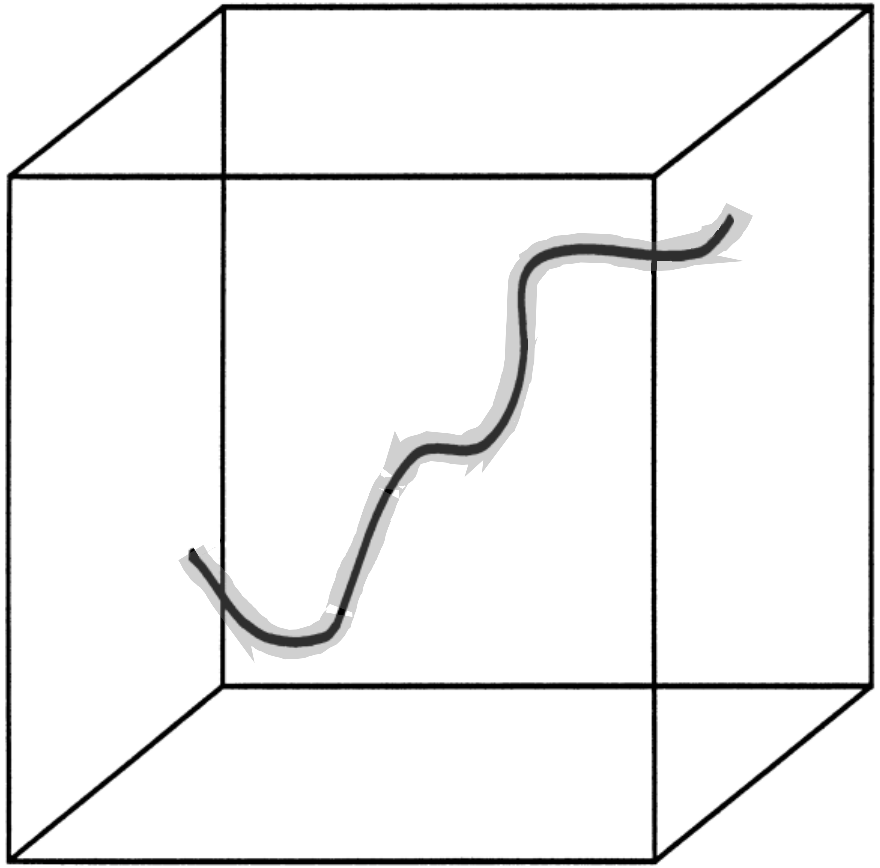
$$\sigma_{ij,j} = 0$$

$$c_{ijkl}U^{e\parallel}_{kl,j} + f_i = 0 \qquad \text{with } f_i = c_{ijkl}U^{e\perp}_{kl,j}$$

$$c_{ijkl}w_{k,lj} + f_i = 0 \qquad \text{with } w_{k,l} = U^{e\parallel}_{kl}$$

Solution using the Green's function approach!

Plastic distortion field



Adapted from *Arsenlis, Parks, Acta Mat. (1999)*

Presence of a dislocation => $\bar{\bar{\boldsymbol{U}}}^{p} \neq \boldsymbol{0}$

$$\bar{\bar{\boldsymbol{U}}}^{\parallel} = \bar{\bar{\boldsymbol{U}}}^{e} + \bar{\bar{\boldsymbol{U}}}^{p} = \bar{\bar{\boldsymbol{U}}}^{e\parallel} + \bar{\bar{\boldsymbol{U}}}^{e\perp} + \bar{\bar{\boldsymbol{U}}}^{p\parallel} + \bar{\bar{\boldsymbol{U}}}^{p\perp}$$

$$\Rightarrow \bar{\bar{\boldsymbol{U}}}^{p\perp} = -\bar{\bar{\boldsymbol{U}}}^{e\perp}$$

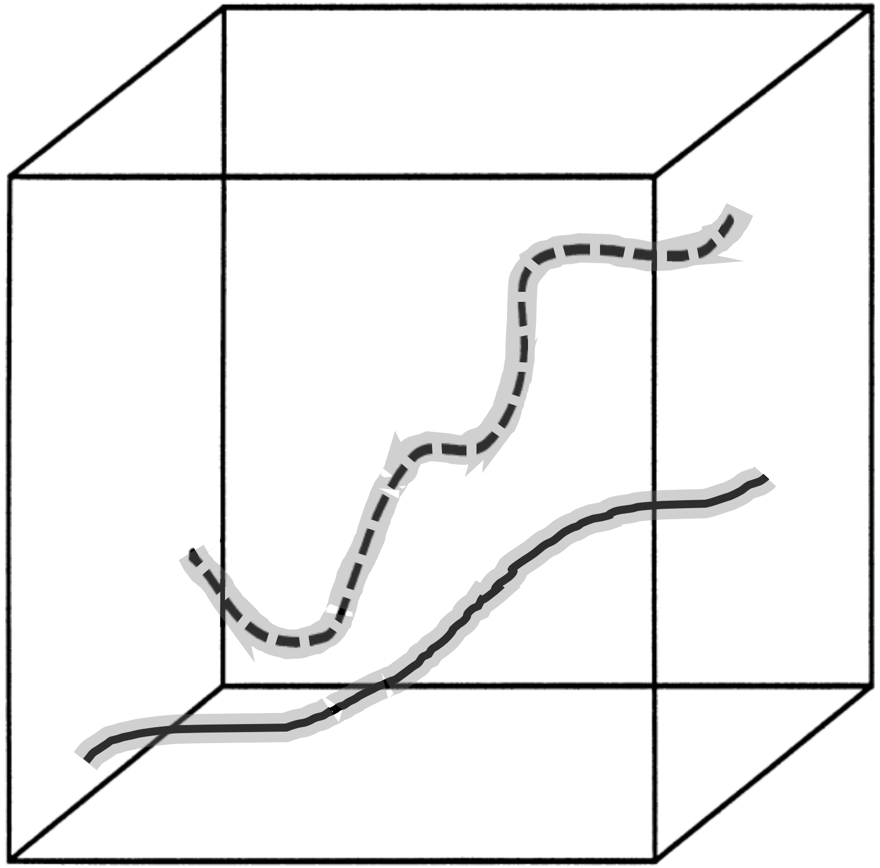
$$\left.\begin{aligned} \mathbf{curl}\, \bar{\bar{\boldsymbol{U}}}^{e\perp} &= \bar{\bar{\boldsymbol{\alpha}}} = -\mathbf{curl}\, \bar{\bar{\boldsymbol{U}}}^{p\perp} \\ \mathbf{div}\, \bar{\bar{\boldsymbol{U}}}^{e\perp} &= \boldsymbol{0} = \mathbf{div}\, \bar{\bar{\boldsymbol{U}}}^{p\perp} \end{aligned}\right\} \text{In } V$$

$$\bar{\bar{\boldsymbol{U}}}^{e\perp} \cdot \overline{\boldsymbol{n}} = \boldsymbol{0} = \bar{\bar{\boldsymbol{U}}}^{p\perp} \cdot \overline{\boldsymbol{n}} \qquad \text{On } S_{body}$$

Given $\bar{\bar{\boldsymbol{\alpha}}}$, $\bar{\bar{\boldsymbol{U}}}^{p\perp}$ obtained using same procedure as $\bar{\bar{\boldsymbol{U}}}^{e\perp}$

Stationary case (no knowledge of history of dislocation motion)
=> Assume $\bar{\bar{\boldsymbol{U}}}^{p\parallel} = \boldsymbol{0}$

Kinematics – transport of a single dislocation



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Conservation of Burgers vector gives

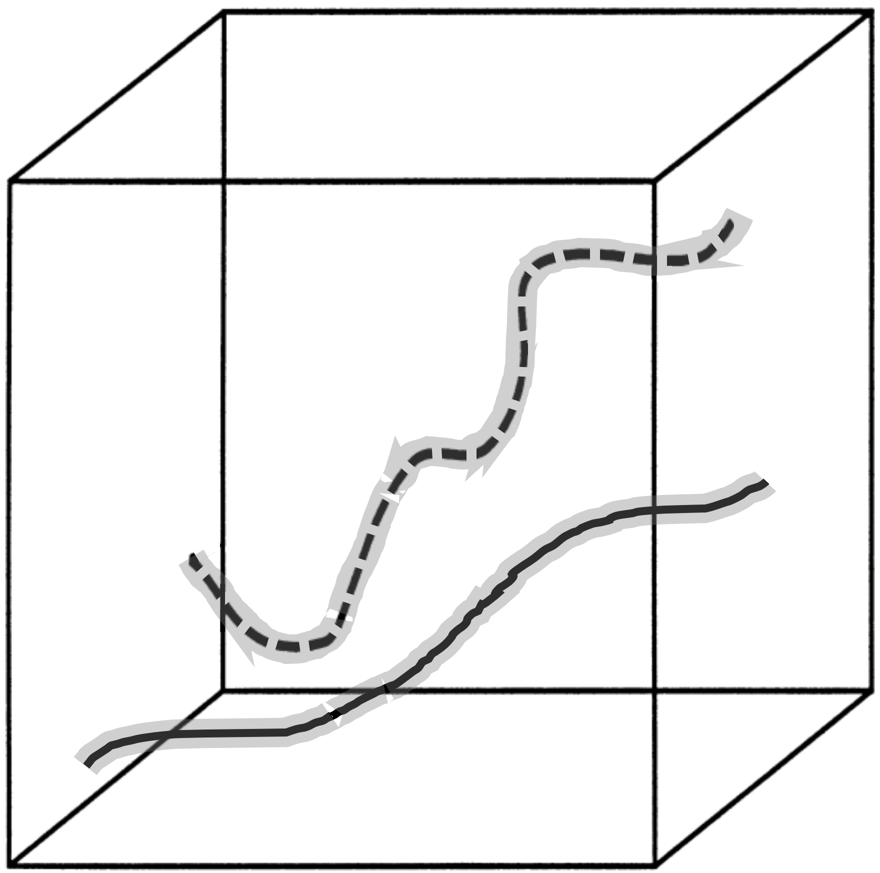
$$\dot{\boldsymbol{b}}^\beta = \frac{\mathrm{d}}{\mathrm{d}t}\int_S \overline{\overline{\boldsymbol{\alpha}}}^\beta \cdot \overline{\boldsymbol{n}}\, dS = \int_S \mathbf{curl}\, \underbrace{\overline{\overline{\boldsymbol{f}}}^\beta}_{\text{Flux}} \cdot \overline{\boldsymbol{n}}\, dS + \int_S \underbrace{\overline{\overline{\boldsymbol{s}}}^\beta}_{\text{Source}} \cdot \overline{\boldsymbol{n}} dS$$

We can prove that $\overline{\overline{\boldsymbol{f}}}^\beta = -\overline{\overline{\boldsymbol{\alpha}}}^\beta \times \overline{\boldsymbol{V}}^\beta$ → Dislocation velocity

Local form: $\dot{\overline{\overline{\boldsymbol{\alpha}}}}^\beta = -\mathbf{curl}\left(\overline{\overline{\boldsymbol{\alpha}}}^\beta \times \overline{\boldsymbol{V}}^\beta\right) + \overline{\overline{\boldsymbol{s}}}^\beta$ – (Acharya 2001)

Question: How to obtain $\overline{\boldsymbol{V}}^\beta$?

Dislocation velocity – 2nd law of thermodynamics



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Power dissipated (Acharya 2003)

$$D = \int_V \bar{\bar{\boldsymbol{\sigma}}} : \dot{\bar{\bar{\boldsymbol{U}}}}^p \, dV = \int_V \sum_\beta \overline{\boldsymbol{F}}^\beta \cdot \overline{\boldsymbol{V}}^\beta \, dV \geq 0$$

With $\overline{\boldsymbol{F}}^\beta = \bar{\bar{\boldsymbol{\sigma}}} \cdot \bar{\boldsymbol{b}}^\beta \times \bar{\boldsymbol{l}}^\beta$ (Peach-Koehler force)

Question: How to obtain $\overline{\boldsymbol{V}}^\beta$?
Answer: In theory, all $\overline{\boldsymbol{V}}^\beta$ that satisfy $\int_V \sum_\beta \overline{\boldsymbol{F}}^\beta \cdot \overline{\boldsymbol{V}}^\beta \, dV \geq 0$ are admissible.

Simplest expression: $\overline{\boldsymbol{V}}^\beta = \frac{1}{B^\beta} \overline{\boldsymbol{F}}^\beta$ with $B^\beta > 0$

Isothermal and adiabatic Elasto-plastic dynamic theory of dislocation fields (Acharya 2003)

$$\left.\begin{aligned}\mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{e\perp} &= \overline{\overline{\boldsymbol{\alpha}}} = -\mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{p\perp}\\ \mathbf{div}\,\overline{\overline{\boldsymbol{U}}}^{e\perp} &= \mathbf{0} = \mathbf{div}\,\overline{\overline{\boldsymbol{U}}}^{p\perp}\end{aligned}\right\}\quad \text{In } V$$

$$\overline{\overline{\boldsymbol{U}}}^{e\perp}\cdot\overline{\boldsymbol{n}} = \mathbf{0} = \overline{\overline{\boldsymbol{U}}}^{p\perp}\cdot\overline{\boldsymbol{n}} \qquad \text{On } S_{body}$$

– Incompatible elastic distortion and plastic distortion

$$\mathbf{div}\,\overline{\overline{\boldsymbol{\sigma}}} = \rho\ddot{\overline{\boldsymbol{u}}}$$

$$\overline{\overline{\boldsymbol{\sigma}}} = \overline{\overline{\overline{\overline{\boldsymbol{C}}}}}:\left(\overline{\overline{\boldsymbol{U}}}^{\parallel} - \overline{\overline{\boldsymbol{U}}}^{p\parallel} - \overline{\overline{\boldsymbol{U}}}^{p\perp}\right)$$

– dynamic equilibrium and elastic constitutive law

$$\overline{\boldsymbol{u}} = \overline{\boldsymbol{u}}^{d} \qquad \text{On } S_{body}^{d}$$

$$\overline{\boldsymbol{t}} = \overline{\overline{\boldsymbol{\sigma}}}\cdot\overline{\boldsymbol{n}} \qquad \text{On } S_{body}^{t}$$

– Dirichlet and Neumann boundary conditions

$$\dot{\overline{\overline{\boldsymbol{\alpha}}}}^{\beta} = -\mathbf{curl}\left(\overline{\overline{\boldsymbol{\alpha}}}^{\beta}\times\overline{\boldsymbol{V}}^{\beta}\right) + \overline{\overline{\boldsymbol{s}}}^{\beta}$$

– Dislocation transport

$$\overline{\boldsymbol{V}}^{\beta} = \frac{1}{B^{\beta}}\overline{\boldsymbol{F}}^{\beta} = \frac{1}{B^{\beta}}\left(\overline{\overline{\boldsymbol{\sigma}}}\cdot\overline{\boldsymbol{b}}^{\beta}\times\overline{\boldsymbol{l}}^{\beta}\right)$$

– Dislocation velocity

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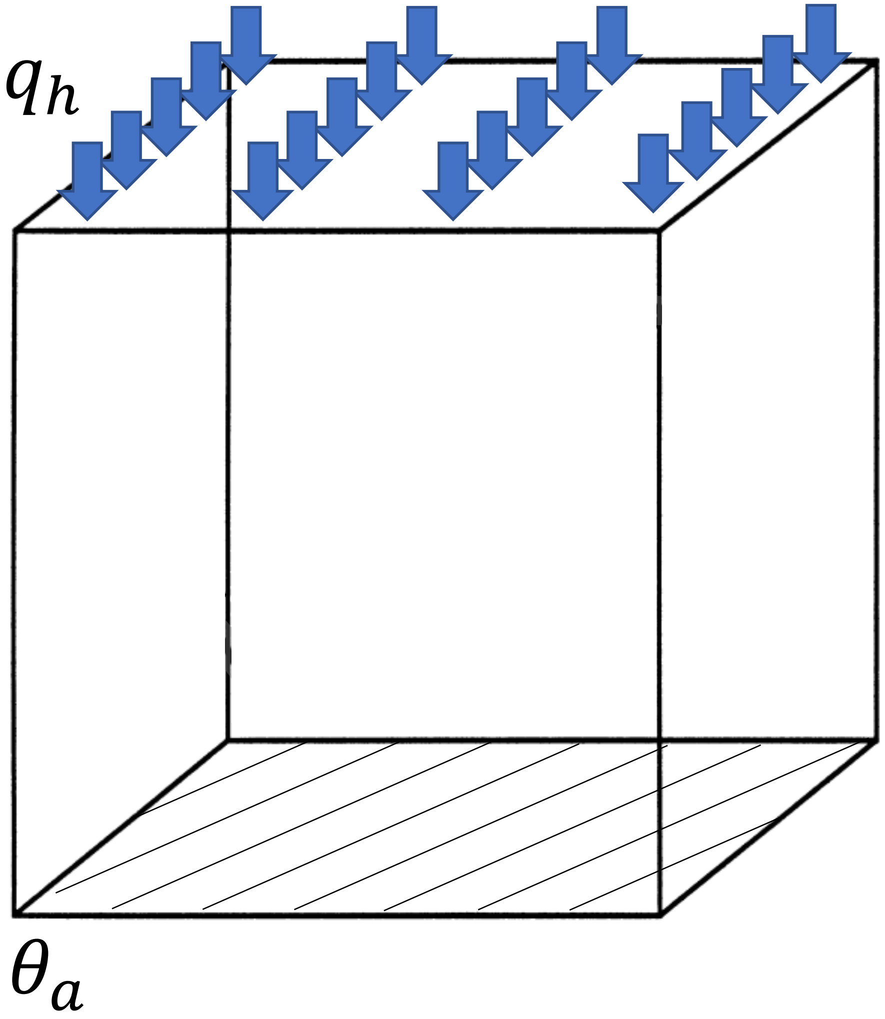
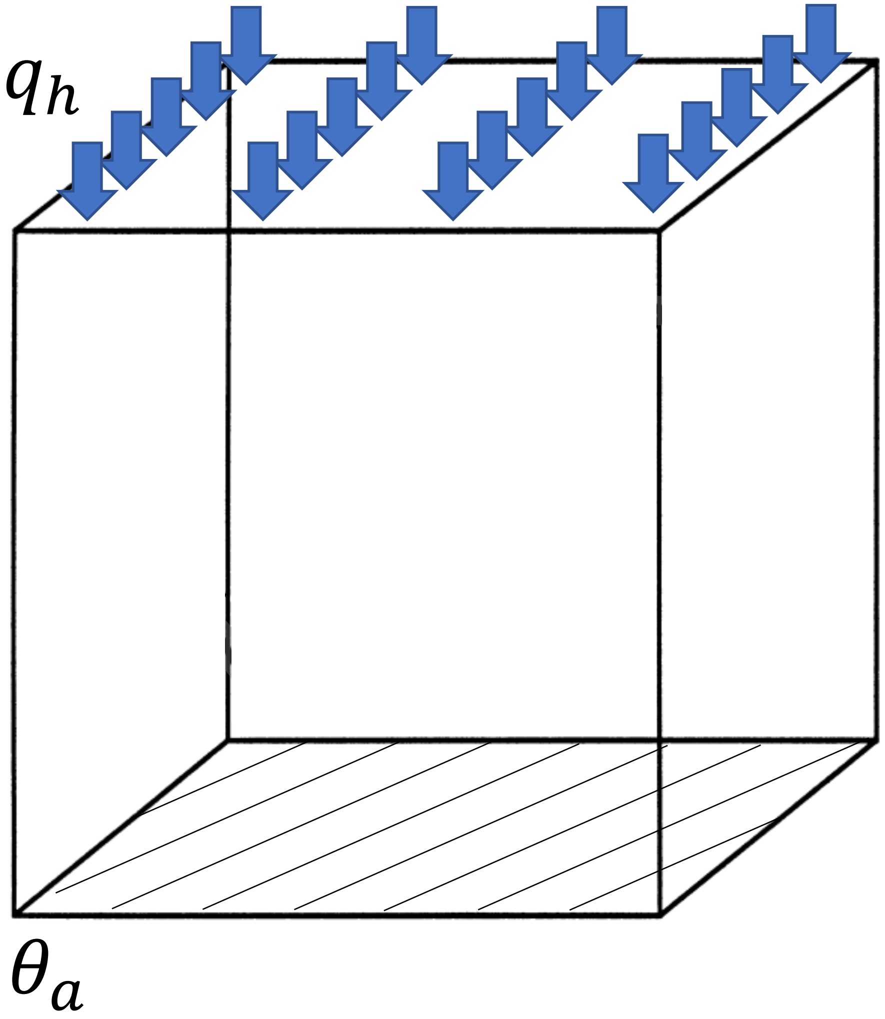
Theory of heat conduction



Boundary conditions

Temperature	$\theta = \theta_a$	On S^{θ}_{body}
Heat flux	$q_h = \overline{\boldsymbol{q}} \cdot \overline{\boldsymbol{n}}$	On S^{q}_{body}

Theory of heat conduction



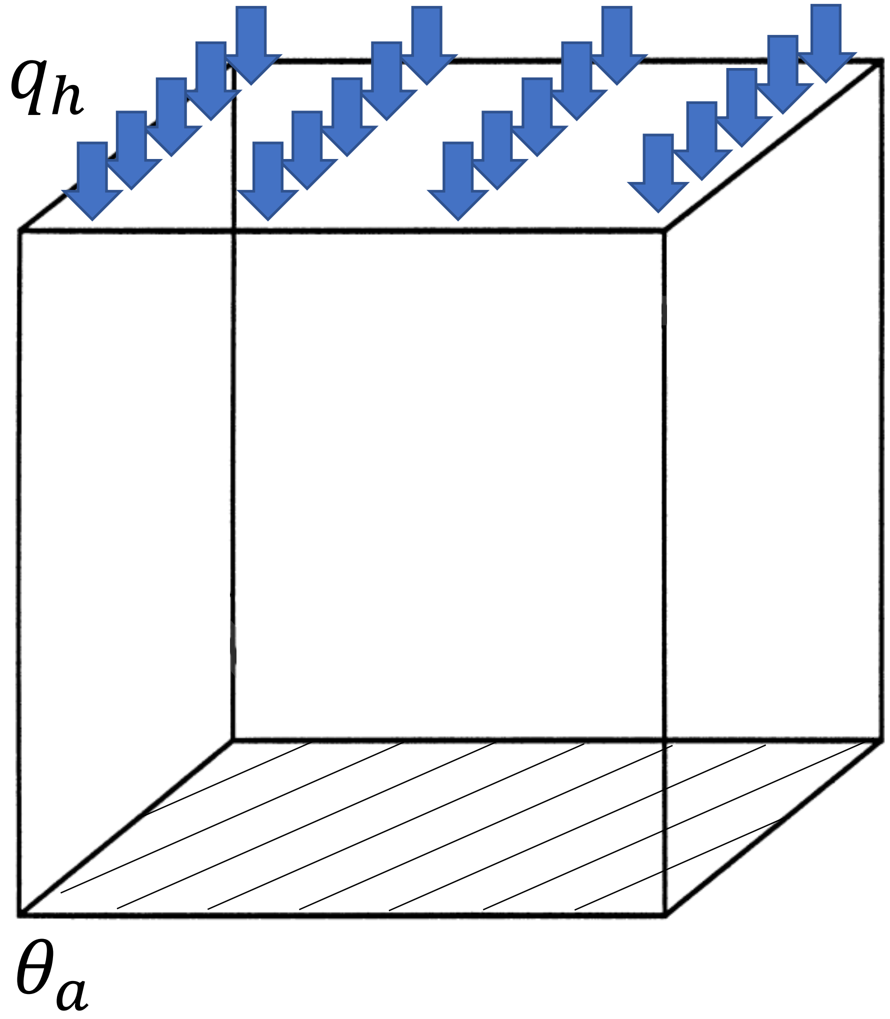
Boundary conditions

Temperature $\theta = \theta_a$ On S_{body}^{θ}

Heat flux $q_h = \overline{\boldsymbol{q}} \cdot \overline{\boldsymbol{n}}$ On S_{body}^{q}

1st law: $\underbrace{\rho c_v \dot{\theta}}_{\text{Internal energy change}} = -\text{div}\,\overline{\boldsymbol{q}} + \underbrace{\rho r}_{\text{Heat loss}}$

Theory of heat conduction



Boundary conditions

Temperature	$\theta = \theta_a$	On S^{θ}_{body}
Heat flux	$q_h = \overline{\boldsymbol{q}} \cdot \overline{\boldsymbol{n}}$	On S^{q}_{body}

1st law: $\underbrace{\rho c_v \dot{\theta}}_{\text{Internal energy change}} = -\mathrm{div}\, \overline{\boldsymbol{q}} + \underbrace{\rho r}_{\text{Heat loss}}$

2nd law: $D = -\int_V \overline{\boldsymbol{q}} \cdot \overline{\boldsymbol{\nabla}\theta}\, dV \geq 0$

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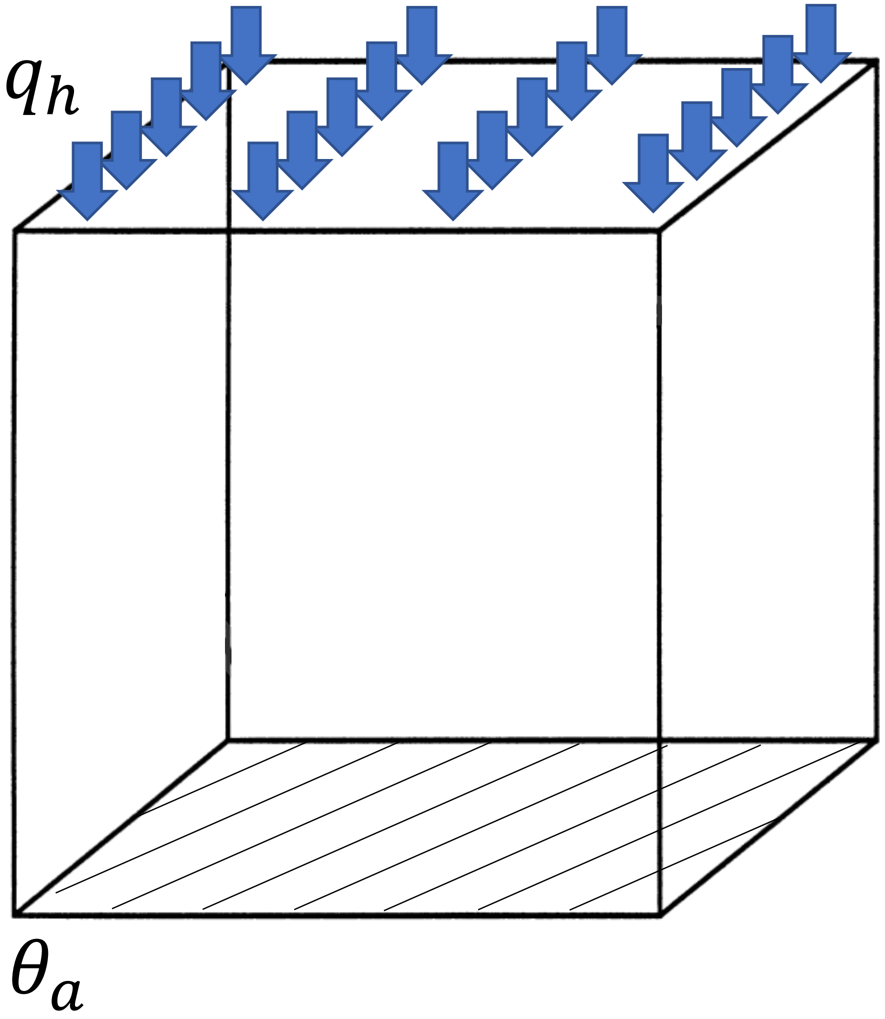

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In theory, all $\overline{\boldsymbol{q}}$ that satisfy $-\int_V \overline{\boldsymbol{q}} \cdot \overline{\boldsymbol{\nabla}\theta}\, dV \geq 0$ are admissible.

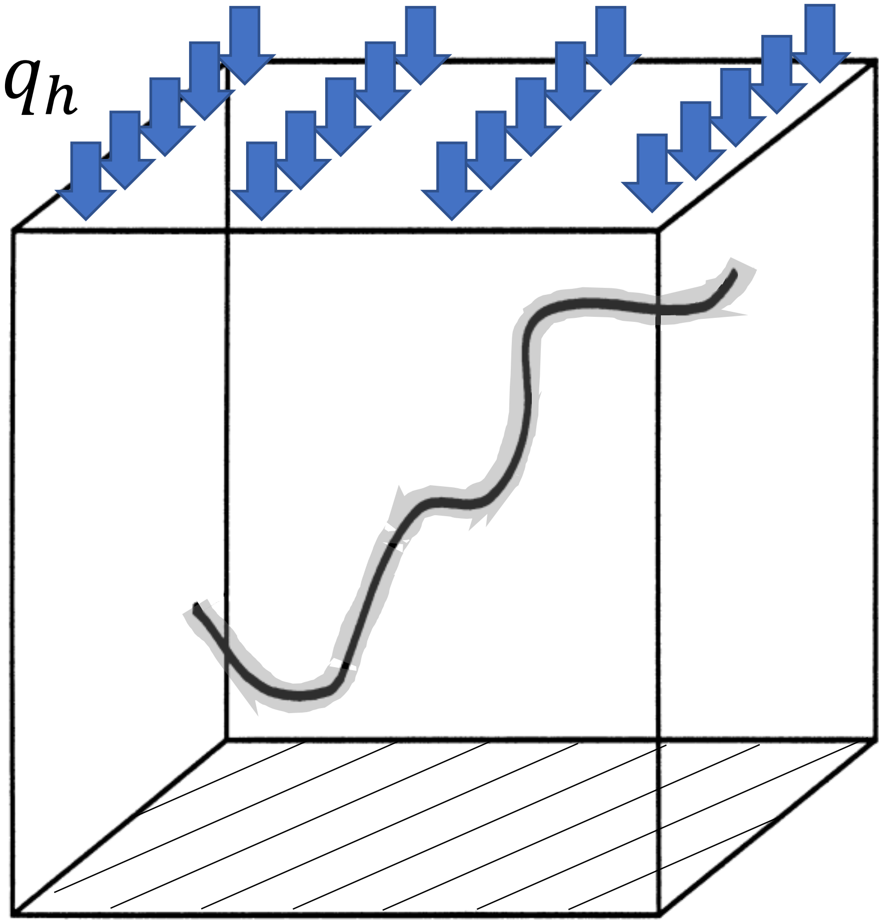
Simplest expression: $\underbrace{\overline{\boldsymbol{q}} = -\overline{\overline{\boldsymbol{K}}} \cdot \overline{\boldsymbol{\nabla}\theta}}_{\text{Fourier law of heat conduction}}$ with $\overline{\overline{\boldsymbol{K}}}$ positive definite

The Thermal Field Dislocation Mechanics (T-FDM) model

Upadhyay, M. V., On the thermo-mechanical theory of field dislocations in transient heterogeneous temperature fields, *Journal of the Mechanics and Physics of Solids,* 105 (2020) 104150

- Development
  - The isothermal and adiabatic FDM model
  - Heat conduction
  - The new T-FDM model
- Model assumptions and impact on AM modelling

Theory of dislocation fields in a steady-state heterogeneous temperature field: Deformation fields

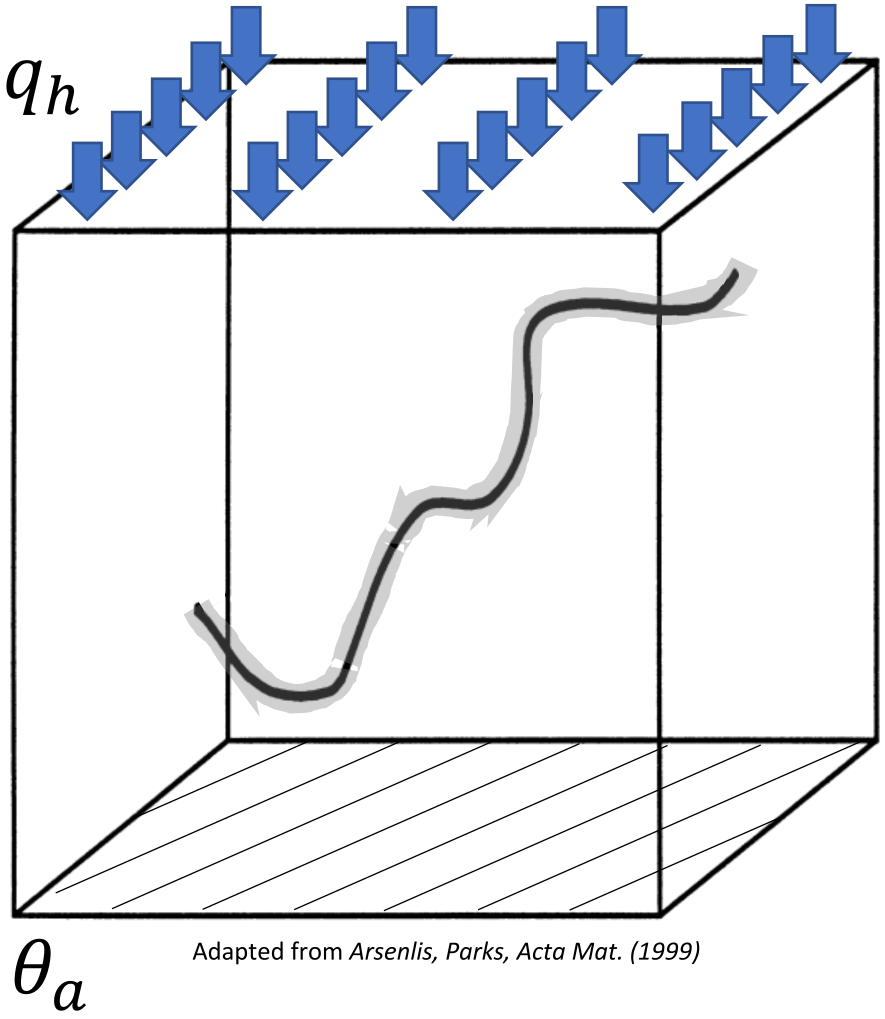


Adapted from *Arsenlis, Parks, Acta Mat. (1999)*

Presence of a heterogeneous temperature field

$$\overline{\overline{\boldsymbol{U}}}^{\parallel} = \overline{\overline{\boldsymbol{U}}}^{e} + \overline{\overline{\boldsymbol{U}}}^{p} + \overline{\overline{\boldsymbol{\varepsilon}}}^{\theta} = \overline{\overline{\boldsymbol{U}}}^{e\parallel} + \overline{\overline{\boldsymbol{U}}}^{e\perp} + \overline{\overline{\boldsymbol{U}}}^{p\parallel} + \overline{\overline{\boldsymbol{U}}}^{p\perp} + ???$$

Theory of dislocation fields in a steady-state heterogeneous temperature field: Deformation fields



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Stokes-Helmholtz decomposition of $\overline{\overline{\boldsymbol{\varepsilon}}}^{\theta}$

$\overline{\overline{\boldsymbol{\varepsilon}}}^{\theta} = \overline{\overline{\boldsymbol{U}}}^{\theta\parallel} + \overline{\overline{\boldsymbol{U}}}^{\theta\perp}$

$\overline{\overline{\boldsymbol{U}}}^{\theta\parallel}$, $\overline{\overline{\boldsymbol{U}}}^{\theta\perp}$ can be asymmetric

They must satisfy $\overline{\overline{\boldsymbol{U}}}^{\theta\parallel} + \overline{\overline{\boldsymbol{U}}}^{\theta\perp} = \left(\overline{\overline{\boldsymbol{U}}}^{\theta\parallel} + \overline{\overline{\boldsymbol{U}}}^{\theta\perp}\right)^{\mathrm{T}}$

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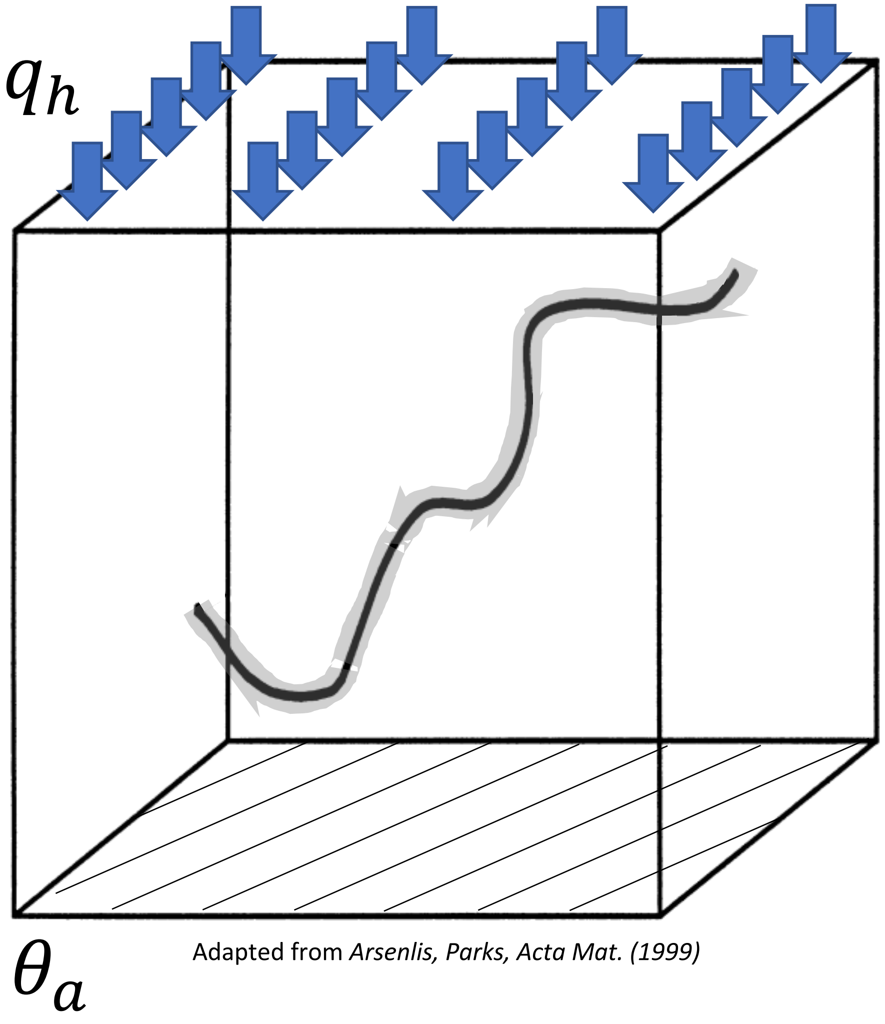

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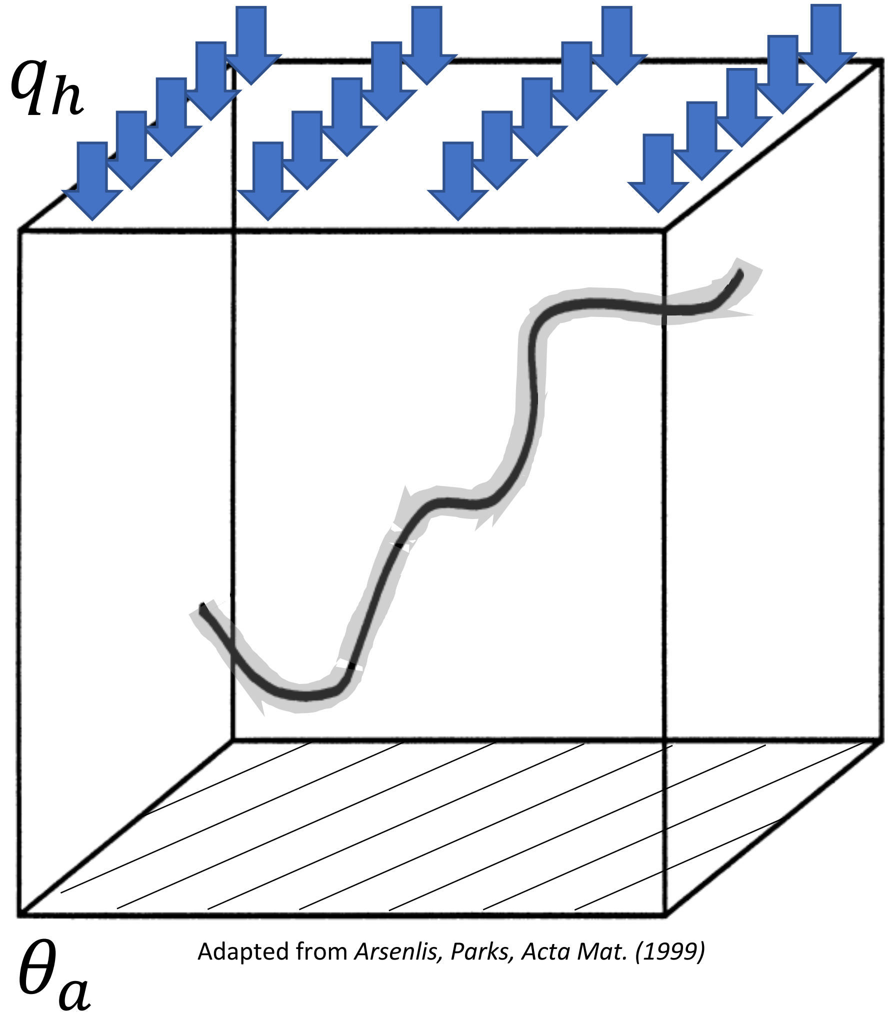
$\overline{\overline{\boldsymbol{U}}}^{e\perp} = -\overline{\overline{\boldsymbol{U}}}^{p\perp} - \overline{\overline{\boldsymbol{U}}}^{\theta\perp}$

Incompatible plastic and thermal distortions contribute to incompatible elastic distortion

Theory of dislocation fields in a steady-state heterogeneous temperature field: Deformation fields



Adapted from *Arsenlis, Parks, Acta Mat. (1999)*

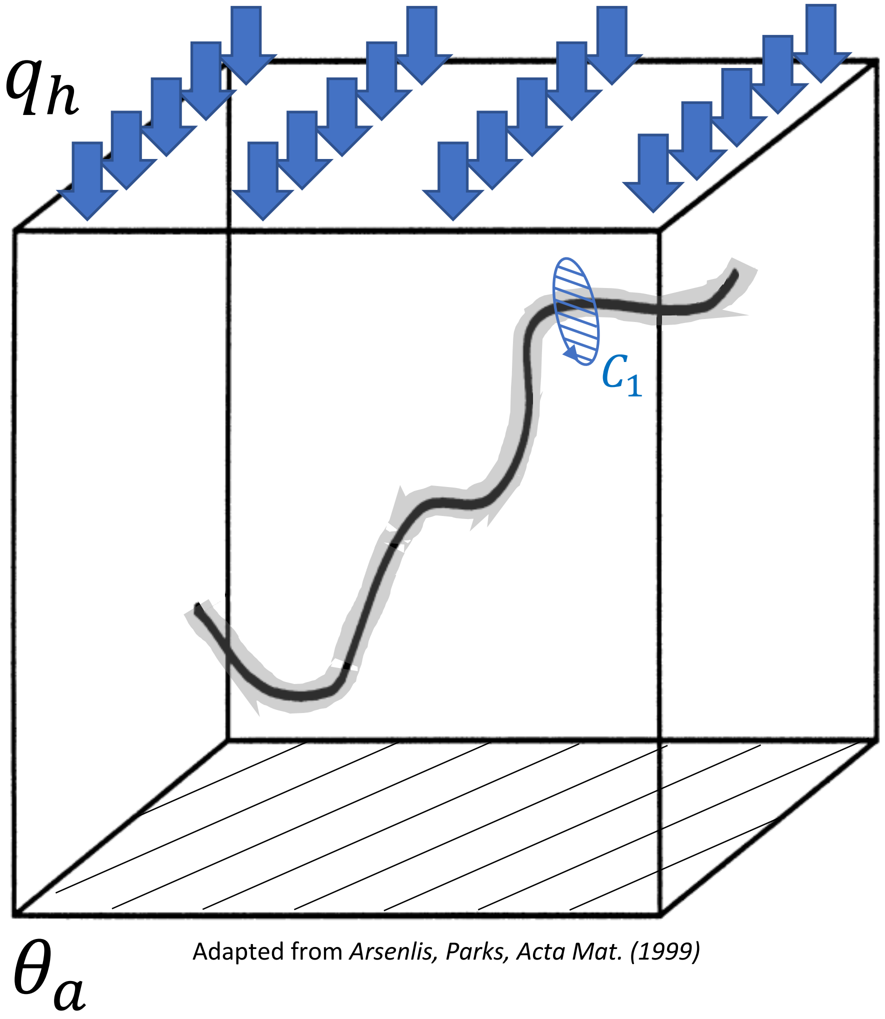
For applications, use empirical formula

$$\overline{\overline{\boldsymbol{\varepsilon}}}^{\theta} = \overline{\overline{\boldsymbol{\gamma}}}(\theta - \theta_0)$$

So what is the point of $\overline{\overline{\boldsymbol{\varepsilon}}}^{\theta} = \overline{\overline{\boldsymbol{U}}}^{\theta\parallel} + \overline{\overline{\boldsymbol{U}}}^{\theta\perp}$?

- Volumetric condition: $\mathbf{div}\ \overline{\overline{\boldsymbol{U}}}^{\theta\perp} = \mathbf{0}$
- Boundary condition: $\overline{\overline{\boldsymbol{U}}}^{\theta\perp} \cdot \overline{\boldsymbol{n}} = \mathbf{0}$

Theory of dislocation fields in a steady-state heterogeneous temperature field: Defect character



Adapted from *Arsenlis, Parks, Acta Mat. (1999)*

Single dislocation – Burgers vector

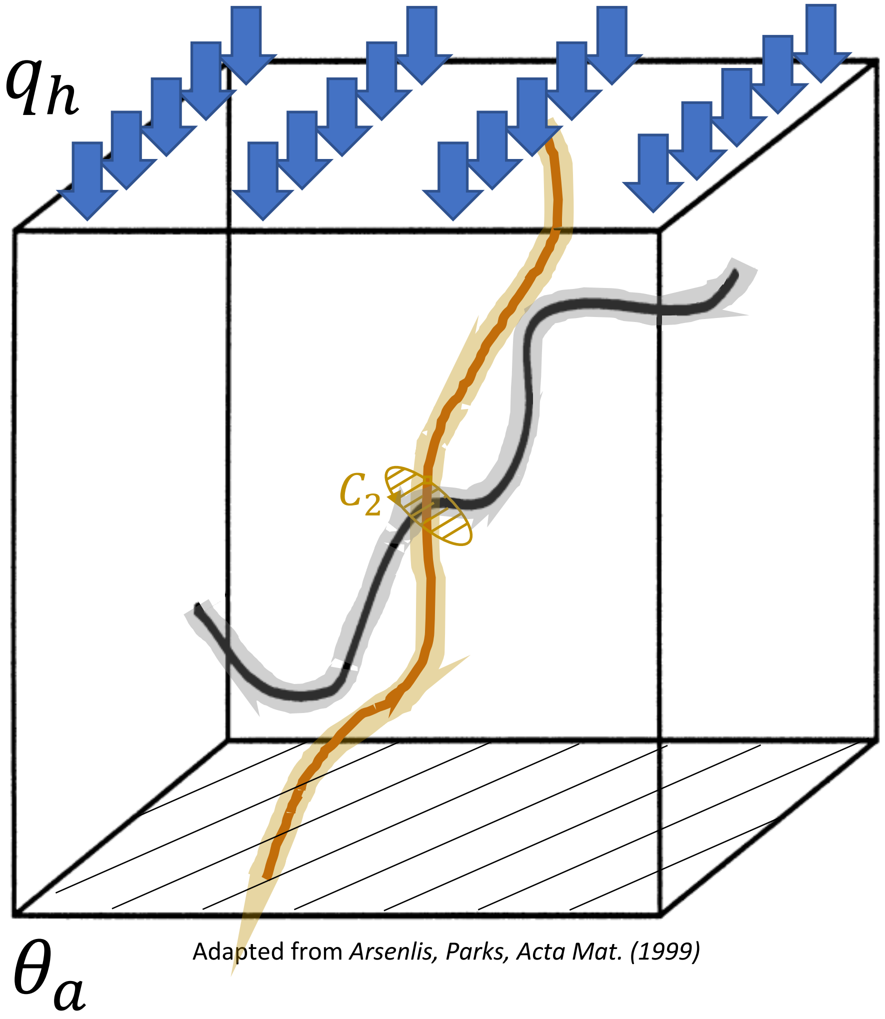
$$\bar{\boldsymbol{b}} = \int_{S_1} \overbrace{\textbf{curl}\, \bar{\bar{\boldsymbol{U}}}^{e\perp}}^{\bar{\bar{\boldsymbol{\alpha}}}} \cdot \bar{\boldsymbol{n}}\, dS$$

$$= \int_{S_1} \underbrace{-\textbf{curl}\, \bar{\bar{\boldsymbol{U}}}^{p\perp}}_{\bar{\bar{\boldsymbol{\alpha}}}^{p,\beta}} \cdot \bar{\boldsymbol{n}}\, dS + \int_{S_1} \underbrace{-\textbf{curl}\, \bar{\bar{\boldsymbol{U}}}^{\theta\perp}}_{\bar{\bar{\boldsymbol{\alpha}}}^{\theta}} \cdot \bar{\boldsymbol{n}}\, dS$$

$$\bar{\bar{\boldsymbol{\alpha}}} = \bar{\bar{\boldsymbol{\alpha}}}^{p,\beta} + \bar{\bar{\boldsymbol{\alpha}}}^{\theta}$$

Nye's tensor = Dislocation density tensor + Thermal quasi-dislocation density tensor (Kröner 1958)

Theory of dislocation fields in a steady-state heterogeneous temperature field: Defect character



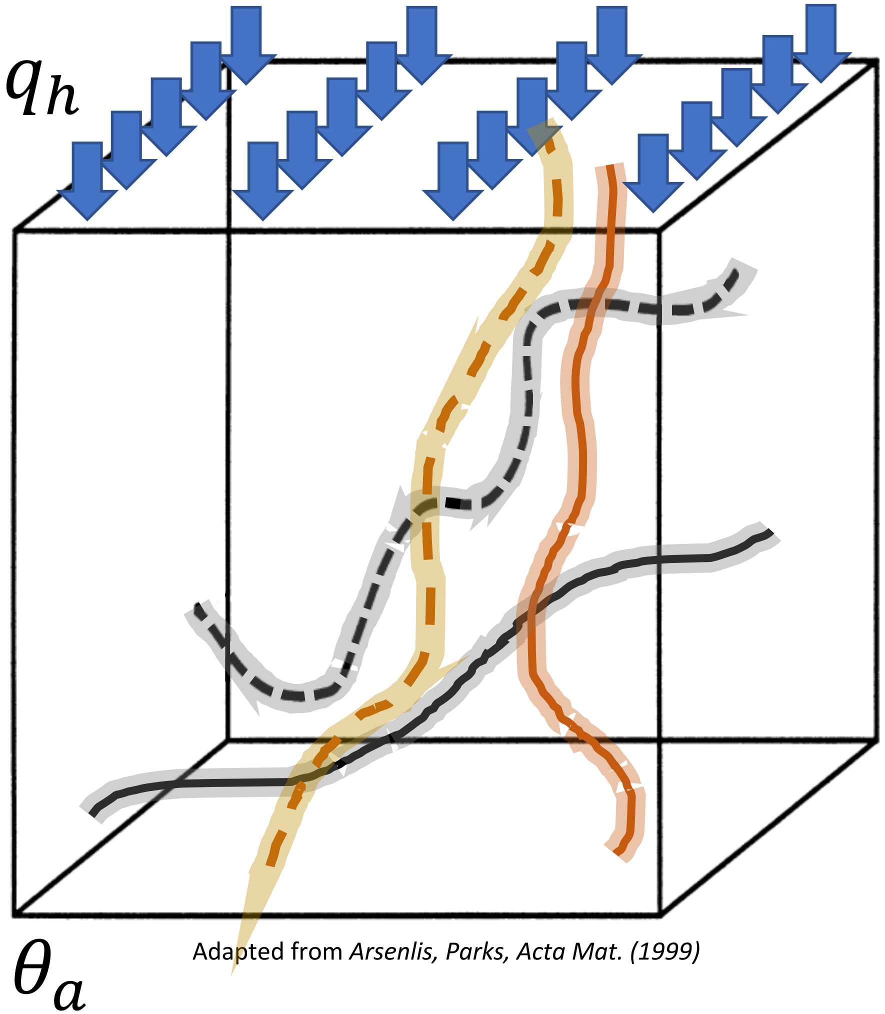
Adapted from *Arsenlis, Parks, Acta Mat. (1999)*

Multiple dislocations

$$\bar{\bar{\boldsymbol{\alpha}}} = \sum_{\beta} \bar{\bar{\boldsymbol{\alpha}}}^{p,\beta} + \bar{\bar{\boldsymbol{\alpha}}}^{\theta}$$

Nye's tensor — Polar dislocation density — Thermal quasi-dislocation density

Kinematics of dislocations in transient heterogeneous temperature fields



Adapted from *Arsenlis, Parks, Acta Mat. (1999)*

Polar dislocation density:

$$\dot{\overline{\overline{\alpha}}}^{p,\beta} = \mathbf{curl}\left(\overline{\overline{\alpha}}^{p,\beta} \times \overline{V}^{\beta}\right) + \overline{\overline{S}}^{p,\beta}$$

Thermal quasi-dislocations:

$$\dot{\overline{\overline{\alpha}}}^{\theta} = \nabla \times \dot{\overline{\overline{\varepsilon}}}^{\theta} \approx -\overline{\overline{\gamma}} \cdot \left[\nabla \dot{\theta} \cdot \overline{\overline{\overline{X}}}\right]$$

3rd order Levi-Civita permutation tensor

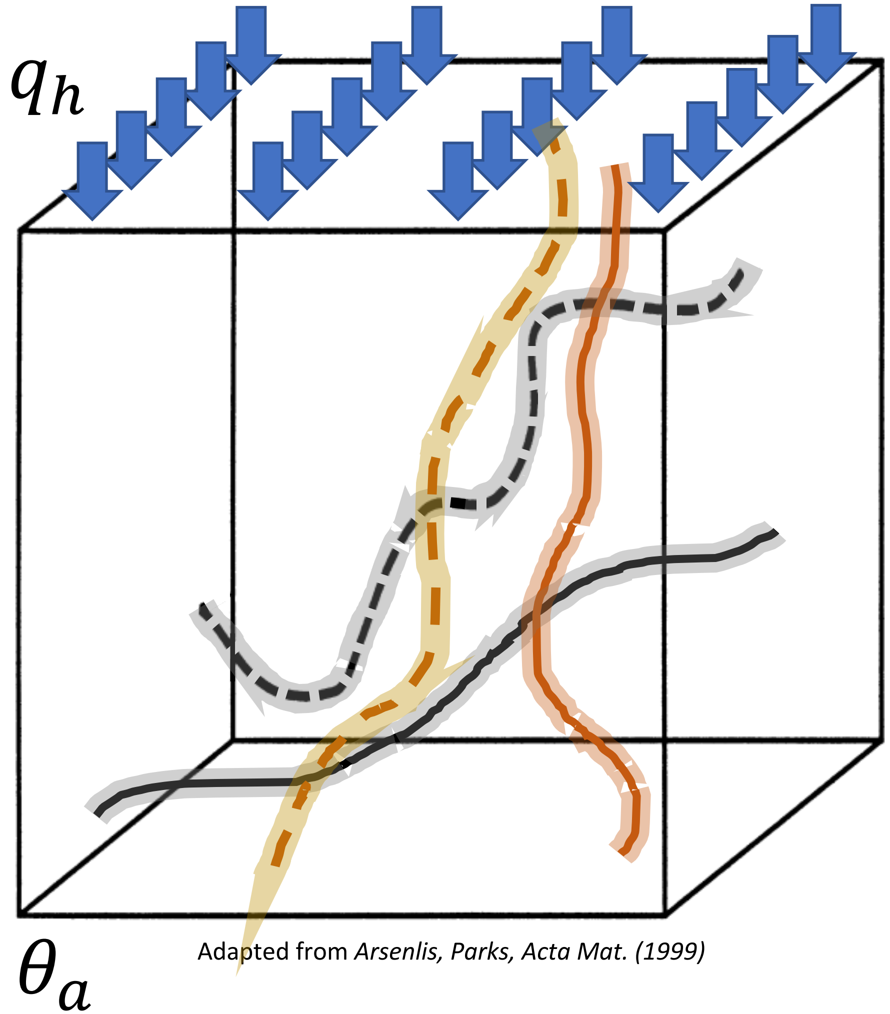
Nye's tensor:

$$\dot{\overline{\overline{\alpha}}} = \mathbf{curl}\, \dot{\overline{\overline{U}}}^{e\perp} = \sum_{\beta}\left(\mathbf{curl}\left(\overline{\overline{\alpha}}^{p,\beta} \times \overline{V}^{\beta}\right) + \overline{\overline{S}}^{p,\beta}\right) + \dot{\overline{\overline{\alpha}}}^{\theta}$$

- Absence of dislocations => Temperature changes result in evolution of $\overline{\overline{\alpha}}$ and $\overline{\overline{U}}^{e\perp}$
- Presence of dislocations
  - Temperature changes can be accommodated by dislocation density evolution without change to $\overline{\overline{\alpha}}$ and $\overline{\overline{U}}^{e\perp}$

  => dislocation structures could form during rapid cooling without change to stress fields

Thermo-mechanical aspects of dislocation fields in transient temperature changes: Temperature evolution



Adapted from *Arsenlis, Parks, Acta Mat. (1999)*

First law:

$$\rho\dot{u} = -\overline{\nabla}\cdot\overline{\boldsymbol{q}} + \overline{\overline{\boldsymbol{\sigma}}}:\dot{\overline{\overline{\boldsymbol{\varepsilon}}}} + \rho r$$

Second law (Clausius Duhem inequality):

$$-\rho\left(\dot{\psi} + s\dot{\theta}\right) + \overline{\overline{\boldsymbol{\sigma}}}:\dot{\overline{\overline{\boldsymbol{\varepsilon}}}} - \frac{1}{\theta}\left(\overline{\boldsymbol{q}}\cdot\overline{\nabla}\theta\right) \geq 0$$

$$-\overline{\overline{\boldsymbol{K}}}\cdot\overline{\nabla}\theta$$

Free energy density evolution:

$$\dot{\psi} = \frac{\partial\psi}{\partial\left(\overline{\overline{\boldsymbol{\varepsilon}}} - \overline{\overline{\boldsymbol{\varepsilon}}}^p\right)}:\left(\dot{\overline{\overline{\boldsymbol{\varepsilon}}}} - \dot{\overline{\overline{\boldsymbol{\varepsilon}}}}^p\right) + \frac{\partial\psi}{\partial\theta}\dot{\theta}$$

Finally,

$$\rho c_\varepsilon\dot{\theta} = \overline{\nabla}\cdot\left(\overline{\overline{\boldsymbol{K}}}\cdot\overline{\nabla}\theta\right) + \overline{\overline{\boldsymbol{\sigma}}}:\dot{\overline{\overline{\boldsymbol{\varepsilon}}}}^p - \theta\overline{\overline{\boldsymbol{\gamma}}}:\overline{\overline{\overline{\overline{\boldsymbol{C}}}}}:\left(\dot{\overline{\overline{\boldsymbol{\varepsilon}}}} - \dot{\overline{\overline{\boldsymbol{\varepsilon}}}}^p\right) + \rho r$$

=> Dislocation motion will result in temperature changes

Dynamics of dislocation fields in transient heterogeneous temperature fields

$$\begin{aligned} \mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{e\perp} &= \overline{\overline{\boldsymbol{\alpha}}} = -\mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{p\perp} - \mathbf{curl}\,\overline{\overline{\boldsymbol{U}}}^{\theta\perp} \\ \mathbf{div}\,\overline{\overline{\boldsymbol{U}}}^{e\perp} &= \mathbf{div}\,\overline{\overline{\boldsymbol{U}}}^{p\perp} = \mathbf{div}\,\overline{\overline{\boldsymbol{U}}}^{\theta\perp} = \mathbf{0} \end{aligned} \quad \text{In } V$$

$$\overline{\overline{\boldsymbol{U}}}^{e\perp}\cdot\overline{\boldsymbol{n}} = \overline{\overline{\boldsymbol{U}}}^{p\perp}\cdot\overline{\boldsymbol{n}} = \overline{\overline{\boldsymbol{U}}}^{\theta\perp}\cdot\overline{\boldsymbol{n}} = \mathbf{0} \qquad \text{On } S_{body}$$

– Incompatible elastic distortion and plastic distortion

$$\mathbf{div}\,\overline{\overline{\boldsymbol{\sigma}}} = \rho\ddot{\overline{\boldsymbol{u}}}$$

$$\overline{\overline{\boldsymbol{\sigma}}} = \overline{\overline{\overline{\overline{\boldsymbol{c}}}}}:\left(\overline{\overline{\boldsymbol{U}}} - \overline{\overline{\boldsymbol{U}}}^{p\parallel} - \overline{\overline{\boldsymbol{U}}}^{p\perp}\right) - \overline{\overline{\overline{\overline{\boldsymbol{c}}}}}:\overline{\overline{\boldsymbol{\gamma}}}(\theta - \theta_0)$$

– dynamic equilibrium and elastic constitutive law

$$\overline{\boldsymbol{u}} = \overline{\boldsymbol{u}}^d \quad \text{On } S^d_{body} \qquad \theta = \hat{\theta} \quad \text{On } S^\theta_{body}$$

$$\overline{\boldsymbol{t}} = \overline{\overline{\boldsymbol{\sigma}}}\cdot\overline{\boldsymbol{n}} \quad \text{On } S^t_{body} \qquad q = \overline{\boldsymbol{q}}^h\cdot\overline{\boldsymbol{n}} \quad \text{On } S^q_{body}$$

– Dirichlet and Neumann boundary conditions

$$\dot{\overline{\overline{\boldsymbol{\alpha}}}} = \sum_{\boldsymbol{\beta}}\left[-\mathbf{curl}\left(\overline{\overline{\boldsymbol{\alpha}}}^{p,\beta}\times\overline{\boldsymbol{v}}^{\beta}\right) + \overline{\overline{\boldsymbol{S}}}^{p,\beta}\right] + \dot{\overline{\overline{\boldsymbol{\alpha}}}}^{\theta}$$

– Dislocation and thermal-quasi dislocation evolution

$$\overline{\boldsymbol{V}}^{\beta} = \frac{1}{B^\beta}\overline{\boldsymbol{F}}^{\beta} = \frac{1}{B^\beta}\left(\overline{\overline{\boldsymbol{\sigma}}}\cdot\overline{\boldsymbol{b}}^{\beta}\times\overline{\boldsymbol{l}}^{\beta}\right)$$

– Dislocation velocity

Upadhyay, JMPS 105 (2020) 104150

$$\rho c_\varepsilon\dot{\theta} = \overline{\boldsymbol{\nabla}}\cdot\left(\overline{\overline{\boldsymbol{K}}}\cdot\overline{\boldsymbol{\nabla}}\theta\right) + \overline{\overline{\boldsymbol{\sigma}}}:\dot{\overline{\overline{\boldsymbol{\varepsilon}}}}^p - \theta\overline{\overline{\boldsymbol{\gamma}}}:\overline{\overline{\overline{\overline{\boldsymbol{c}}}}}:\left(\dot{\overline{\overline{\boldsymbol{\varepsilon}}}} - \dot{\overline{\overline{\boldsymbol{\varepsilon}}}}^p\right) + \rho r$$

– Internal energy balance

$$\overline{\boldsymbol{q}} = -\overline{\overline{\boldsymbol{K}}}\cdot\overline{\boldsymbol{\nabla}}\theta$$

– Fourier law of heat conduction

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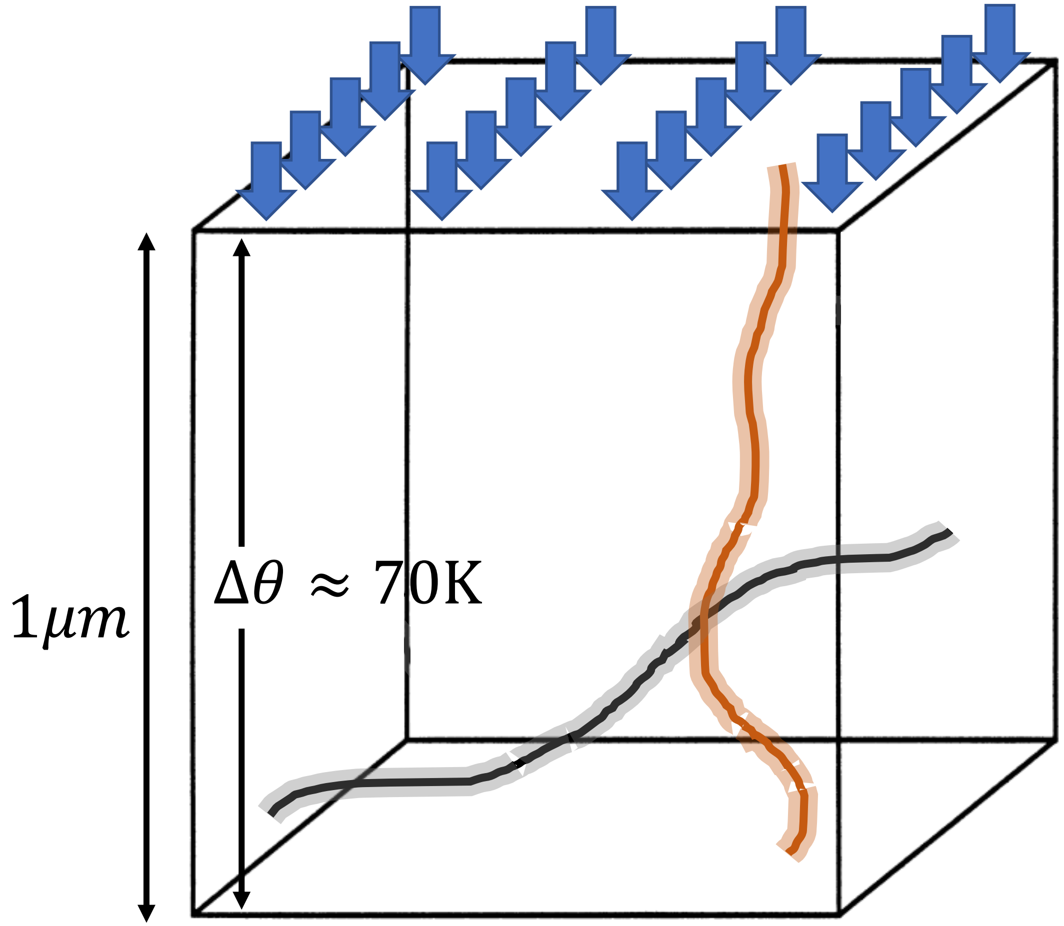
  - Heat conduction
  - The new T-FDM model
- Model assumptions and impact on AM modelling

Model assumptions and impact on AM modeling

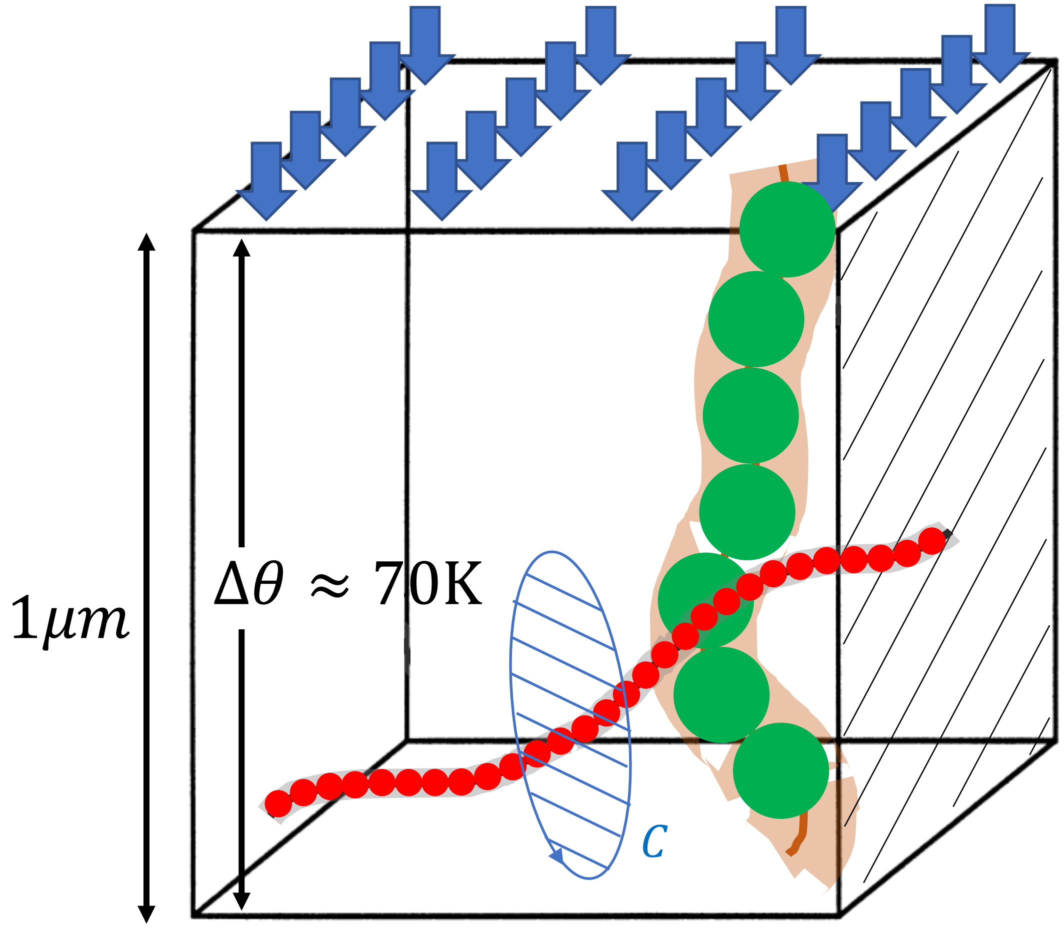


- Local thermodynamic equilibrium
  - Highest $\dot{\theta}$ during SSTC $\approx 10^6\ K/s$
  - In $10^{-12}s$, $\Delta\theta = 10^{-6}K$
  - Atomic fluctuations corresponding to thermal equilibrium for $\Delta t > 10^{-12}s$

  $\Rightarrow$ Thermal equilibrium instantaneously achieved compared to changes in boundary condition

  Model is suitable to simulate DD during AM

Model assumptions and impact on AM modeling



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  Model is suitable to simulate DD during AM

- Need careful treatment during upscaling

  – Too large V or C => non-local temperature effects

Summary

- The thermo-mechanically rigorous T-FDM model captures
  - Isothermal/adiabatic dislocation dynamics

    +
  - Dislocation generation/annihilation/motion/density evolution due to temperature evolution

    +
  - Temperature changes induced by moving dislocations

Upadhyay, M. V., On the thermo-mechanical theory of field dislocations in transient heterogeneous temperature fields, *Journal of the Mechanics and Physics of Solids,* 105 (2020) 104150.

https://doi.org/10.1016/j.jmps.2020.104150