Numerical implementation of Field Dislocation Mechanics with applications in mesoscale simulations

Rajat Arora, Abhishek Arora, Amit Acharya
PI: Amit Acharya

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This renewal proposal is organized as follows: we first present a brief overview of the governing equations of MFDM in section 2. The finite element discretization of the governing equations of the system are presented in 3. We lay out the code structure and the computational algorithm in section 4. We then present the future computation plan and justification of computing resources requested in section 5. Results obtained using previous allocations are presented in the accompanying progress report.

1 Overview

Dislocations, being the primary carriers of plastic deformation, play a pivotal role in determining the strength and mechanical properties of engineering materials. The use of first principles to understand complex dislocation interactions occurring at extremely small spatial and temporal scales has been successful in modeling material behavior. However, the steep computational cost associated with these methods limit the system sizes and simulation times that can be achieved in practice. Hence, a continuum scale 'fundamentally accurate' model that enables a predictive understanding of dislocation-mediated deformation serves a complementary purpose.

Dislocations are understood as line defects that exist in most natural crystalline solids. The nucleations and motions of dislocations are the major mechanism that govern plasticity. The theory of Field Dislocation Mechanics (FDM) is a dislocation based modern continuum mechanics model which has been developed through a series of works, presented by Acharya [Ach01, Ach03, Ach04, Ach10, Ach11] and Acharya and Roy [AR06]. Its basis lies in a kinematically faithful representation of dislocation motion and calculation of internal stress. FDM builds on the pioneering works of Kröner [Krö81], Mura [Mur63], Fox [Fox66], and Willis [Wil67] that almost exclusively develop the static elastic theory of continuously distributed dislocations, and extends this body of work to account for dissipative dislocation transport and nonlinearity due to geometric and crystal elasticity effects. FDM describes dislocation behavior through fields that account for lattice incompatibility. Recent works of Acharya and Zhang [AZ15] and Zhang, et. al., [ZAWB15] demonstrate the ability of FDM in modelling phenomena of atomic scale, such as dislocation annihilation/dissociation, Peierls stress and supersonic dislocations, as well as rupture dynamics at tectonic scales. For crystalline materials, FDM represents defects in the crystal lattice at the atomic scale but a space-time averaged FDM allows simulations at the meso and macro scales [Ach11, AR06]. Therefore, the dislocation density field, which denotes the density of curves carrying a vectorial Burgers' vector attribute, is defined at every modeling scale. Previous works of [Pur09, RA06, AA20b, Aro19, AZA20, AA20a, Aro21], among others, show the process of modeling mesoscopic problems with FDM.

2 Mesoscale Field Dislocation Mechanics with constitutive specifications

This section presents the governing equations, constitutive assumptions, and initial and boundary conditions of finite deformation Mesoscale Field Dislocation Mechanics, the model that is computationally implemented and evaluated in this document. The relevant field equations are summarized briefly:

$$\mathring{\boldsymbol{\alpha}} \equiv (div\,\boldsymbol{v})\boldsymbol{\alpha} + \dot{\boldsymbol{\alpha}} - \boldsymbol{\alpha}\boldsymbol{L}^T = -curl\,(\boldsymbol{\alpha}\times\boldsymbol{V} + \boldsymbol{L}^p) \tag{1a}$$

$$\boldsymbol{W} = \boldsymbol{\chi} + grad\boldsymbol{f}$$

$$\left.\begin{aligned} curl\boldsymbol{W} = curl\boldsymbol{\chi} = -\boldsymbol{\alpha} \\ div\boldsymbol{\chi} = \boldsymbol{0} \end{aligned}\right\} \tag{1b}$$

$$div\left(grad\dot{\boldsymbol{f}}\right) = div\,(\boldsymbol{\alpha}\times\boldsymbol{V} + \boldsymbol{L}^p - \dot{\boldsymbol{\chi}} - \boldsymbol{\chi}\boldsymbol{L}) \tag{1c}$$

$$div\,[\boldsymbol{T}(\boldsymbol{W})] = \begin{cases} \boldsymbol{0} & \text{quasistatic} \\ \rho\,\dot{\boldsymbol{v}} & \text{dynamic.} \end{cases} \tag{1d}$$

In (1), $\boldsymbol{W}$ is the inverse-elastic distortion tensor, $\boldsymbol{\chi}$ is the incompatible part of $\boldsymbol{W}$, $\boldsymbol{f}$ is the plastic position vector, $grad\boldsymbol{f}$ represents the compatible part of $\boldsymbol{W}$, $\boldsymbol{\alpha}$ is the dislocation density tensor, $\boldsymbol{v}$ represents the material velocity field, $\boldsymbol{L} = grad\boldsymbol{v}$ is the velocity gradient, and $\boldsymbol{T}$ is the (symmetric) Cauchy stress tensor, and $\boldsymbol{V}$ is the dislocation velocity field. An important thing to note is that if $\boldsymbol{L}^p = \boldsymbol{0}$ then the system (1) refers to the governing equations of FDM theory; otherwise, it represents the MFDM model. FDM applies to understanding the mechanics of small collections of dislocations, resolved at the scale of individual dislocations. MFDM is a model for mesoscale plasticity with clear connections to microscopic FDM. The fields involved in the MFDM model are space-time averaged counterparts of the fields of FDM ((1) with no $\boldsymbol{L}^p$), with $\boldsymbol{L}^p$ being an emergent additional mesoscale field.

2.1 Constitutive equations for $\boldsymbol{T}$, $\boldsymbol{L}^p$, and $\boldsymbol{V}$

MFDM requires constitutive statements for the stress $\boldsymbol{T}$, the plastic distortion rate $\boldsymbol{L}^p$, and the dislocation velocity $\boldsymbol{V}$. The details of the thermodynamically consistent constitutive formulations are presented in [AA19, Sec. 3.1]. This constitutive structure is summarized below.

Table 1 presents the Cauchy stress expressions for the Saint-Venant-Kirchhoff and a compressible Neo-Hookean material. It also presents the assumed constitutive form of the mesoscopic core energy density (per unit mass) for the material. Table 2 presents the constitutive assumptions for $\boldsymbol{L}^p$ for Crystal and J_2 plasticity models. Table 3 presents the constitutive assumptions for $\boldsymbol{V}$ for Crystal and J_2 plasticity models. Table 4 presents the governing equation for the evolution of material strength g for the two models. The use of $\hat{\gamma}_{sd}$ in (10) stems from the fact that isotropic (or Taylor) hardening is used for the evolution of g on every slip system i.e. $\dot{g}^k = \sum_j^{n_{sl}} h_{kj}|\hat{\gamma}^j|$ with $h_{kj} = \mathsf{I}_{kj}$, where I is an $n_{sl}\times n_{sl}$ square matrix with 1 as all of its entries. Table 5 presents the boudary conditions and the initial conditions for the theory.

All material parameters, except k_0 and l, are part of the constitutive structure of well-accepted models of classical plasticity theory. Our model requires these two extra material parameters beyond

Saint-Venant-Kirchhoff Material	$\phi(\boldsymbol{W}) = \frac{1}{2\rho^*}\boldsymbol{E}^e : \mathbb{C} : \boldsymbol{E}^e$	$\boldsymbol{T} = \boldsymbol{F}^e\left[\mathbb{C} : \boldsymbol{E}^e\right]\boldsymbol{F}^{eT}$ (2)
Neo-Hookean Material	$\phi(\boldsymbol{W}) = \frac{\mu}{2\rho^*}\left(I_1(\boldsymbol{C}^e) - \ln\left(det(\boldsymbol{C}^e)\right)\right)$	$\boldsymbol{T} = \mu(\boldsymbol{F}^e\boldsymbol{F}^{eT} - \boldsymbol{I})$ (3)
Core energy density	$\Upsilon(\boldsymbol{\alpha}) := \frac{1}{2\rho^*}\epsilon\,\boldsymbol{\alpha} : \boldsymbol{\alpha}$	

Table 1: Constitutive choices for elastic energy density, Cauchy stress, and core energy density.

Crystal plasticity	$\hat{\boldsymbol{L}}^p = \boldsymbol{W}\left(\sum_k^{n_{sl}} \hat{\gamma}^k\,\boldsymbol{m}^k \otimes \boldsymbol{n}^k\right)_{sym}$ (4) $\boldsymbol{L}^p = \hat{\boldsymbol{L}}^p + \left(\frac{l^2}{n_{sl}}\sum_k^{n_{sl}}\lvert\hat{\gamma}^k\rvert\right) curl\boldsymbol{\alpha}$ (5) $\hat{\gamma}^k = sgn(\tau^k)\,\hat{\gamma_0}^k\left(\frac{\lvert\tau^k\rvert}{g}\right)^{\frac{1}{m}}$ (6) $\tau^k = \boldsymbol{m}^k \cdot \boldsymbol{T}\boldsymbol{n}^k;\quad \boldsymbol{m}^k = \boldsymbol{F}^e\boldsymbol{m}_0^k;\quad \boldsymbol{n}^k = \boldsymbol{F}^{e-T}\boldsymbol{n}_0^k$
J_2 plasticity	$\hat{\boldsymbol{L}}^p = \hat{\gamma}\boldsymbol{W}\frac{\boldsymbol{T}'}{\lvert\boldsymbol{T}'\rvert};\quad \hat{\gamma} = \hat{\gamma_0}\left(\frac{\lvert\boldsymbol{T}'\rvert}{\sqrt{2}\,g}\right)^{\frac{1}{m}}$ $\boldsymbol{L}^p = \hat{\boldsymbol{L}}^p + l^2\hat{\gamma}\,curl\boldsymbol{\alpha}$ (7)

Table 2: Constitutive choices for plastic strain rate due to SDs $\boldsymbol{L}^p$.

$$T'_{ij} = T_{ij} - \frac{T_{mm}}{3}\delta_{ij};\qquad a_i := \frac{1}{3}T_{mm}\varepsilon_{ijk}F^e{}_{jp}\alpha_{pk};\qquad c_i := \varepsilon_{ijk}T'_{jr}F^e{}_{rp}\alpha_{pk}$$

$$\boldsymbol{d} = \boldsymbol{c} - \left(\boldsymbol{c}\cdot\frac{\boldsymbol{a}}{\lvert\boldsymbol{a}\rvert}\right)\frac{\boldsymbol{a}}{\lvert\boldsymbol{a}\rvert};\qquad \hat{\gamma}_{avg} = \begin{cases}\hat{\gamma} & J_2 \text{ plasticity}\\ \frac{1}{n_{sl}}\sum_k^{n_{sl}}\lvert\hat{\gamma}^k\rvert & \text{Crystal plasticity.}\end{cases}$$

$$\boldsymbol{V} = \zeta\frac{\boldsymbol{d}}{\lvert\boldsymbol{d}\rvert}\quad ;\quad \zeta = \left(\frac{\mu}{g}\right)^2\eta^2\,b\,\hat{\gamma}_{avg} \tag{8}$$

Table 3: Constitutive choices for dislocation velocity $\boldsymbol{V}$.

$$\hat{\gamma}_{sd} = \begin{cases} \hat{\gamma} & J_2 \text{ plasticity} \\ \sum_k^{n_{sl}} |\hat{\gamma}^k| & \text{Crystal plasticity.} \end{cases} \tag{9}$$

$$\dot{g} = \left[\frac{\mu^2 \eta^2 b}{2(g - g_0)} k_0 \left| \boldsymbol{\alpha} \right| + \Theta_0 \left(\frac{g_s - g}{g_s - g_0} \right) \right] \left(\left| \boldsymbol{F}^e \boldsymbol{\alpha} \times \boldsymbol{V} \right| + \hat{\gamma}_{sd} \right) \tag{10}$$

Table 4: Evolution equation for material strength g.

Boundary Conditions	$\boldsymbol{\chi} \cdot \boldsymbol{n} = \boldsymbol{0}$ on $\partial\Omega$ $(grad\dot{\boldsymbol{f}})\boldsymbol{n} = (\boldsymbol{\alpha} \times \boldsymbol{V} + \boldsymbol{L}^p - \dot{\boldsymbol{\chi}} - \boldsymbol{\chi}\boldsymbol{L})\boldsymbol{n}$ on $\partial\Omega$ $(\boldsymbol{\alpha} \times \boldsymbol{V} + \boldsymbol{L}^p) \times \boldsymbol{n} = \boldsymbol{\Phi}$, such that $\boldsymbol{\Phi}\boldsymbol{n} = \boldsymbol{0}$ *Constrained case:* $\boldsymbol{\Phi} = \boldsymbol{0}$ *Unconstrained case:* Specification of $\hat{\boldsymbol{L}^p} \times \boldsymbol{n}$ and $l^2 \hat{\gamma_{sd}} (\boldsymbol{\alpha} \times \boldsymbol{n})$ on the boundary and $\boldsymbol{\alpha}(\boldsymbol{V} \cdot \boldsymbol{n})$ on the inflow boundary
Initial Conditions	$curl\boldsymbol{\chi} = -\boldsymbol{\alpha}$ $div\boldsymbol{\chi} = \boldsymbol{0}$ $div\,[\boldsymbol{T}(\boldsymbol{f}, \boldsymbol{\chi})] = \boldsymbol{0}$ } on Ω (11) $\boldsymbol{\chi}\boldsymbol{n} = \boldsymbol{0}$ $\boldsymbol{T}\boldsymbol{n} = \boldsymbol{t}$ } on $\partial\Omega$ (12) $\boldsymbol{t}$ denotes the statically admissible traction field on the boundary. This determination of $\boldsymbol{\chi}$, $\boldsymbol{f}$, and $\boldsymbol{T}$ for a given dislocation density $\boldsymbol{\alpha}$ on any known configuration will be referred to as the ECDD solve on that configuration. $\dot{\boldsymbol{f}} = \boldsymbol{0}$ at an arbitrarily chosen point.

Table 5: Boundary and initial conditions for the model.

the requirements of classical theory. l (with physical dimensions of length) sets the length scale for the mesoscopic core energy to be effective, and k_0 (non-dimensional) characterizes the plastic flow resistance due to ED. We mention here that the length scale l, introduced in Eq. (5) or (7) as a dimensional consequence of including the core energy, is not responsible for producing enhanced size effects and microstructure in MFDM. Rather, the 'smaller is harder' size effect decreases with increasing magnitude of l since its presence reduces the magnitude of the $\boldsymbol{\alpha}$ field and consequently reduces hardening (10).

3 Variational formulations

Modeling material behavior through the use of MFDM requires the concurrent solution to a coupled nonlinear system of pdes given by (1). To efficiently solve the system for the quasistatic case within a staggered scheme in each time increment as in [RA05, RA06] in the small deformation case, we augment the system (1) with the rate (or incremental) form of the equilibrium equation. This rate form is solved to get the material velocity field $\boldsymbol{v}$ on the domain which can be used to (discretely)

update the geometry of the body. In the absence of body forces and inertia, the statement of local force balance (on the current configuration) w.r.t. any choice of reference configuration can be expressed by

$$Div\boldsymbol{P} = \boldsymbol{0}, \tag{13}$$

where $\boldsymbol{P}$ represents the first Piola-Kirchhoff stress w.r.t. that reference. This implies

$$\dot{\overline{Div\,\boldsymbol{P}}} = \boldsymbol{0} \;\; ; \;\; Div\left[J\,tr(\boldsymbol{L})\,\boldsymbol{T}\boldsymbol{F}^{-T} + J\dot{\boldsymbol{T}}\boldsymbol{F}^{-T} + J\boldsymbol{T}\dot{\overline{\boldsymbol{F}^{-T}}}\right] = \boldsymbol{0},$$

where $J = det(\boldsymbol{F})$ and choosing the reference configuration to be the current one i.e. $\boldsymbol{F} = \boldsymbol{I}$, one obtains [MR75]

$$div\left[tr(\boldsymbol{L})\,\boldsymbol{T} + \dot{\boldsymbol{T}} - \boldsymbol{T}\boldsymbol{L}^T\right] = \boldsymbol{0}. \tag{14}$$

The system (1) is then augmented with Eq. (14) for the quasistatic case. For the dynamic case, the balance of linear momentum can be solved directly to give the material velocity field on the domain.

The FEM formulation and algorithm presented here are independent of the constitutive choices made for $\boldsymbol{L}^p$, $\boldsymbol{V}$, and $\boldsymbol{T}$. We now discuss the numerical schemes to solve the governing equations. A typical time increment between times t^n to t^{n+1} is considered. $(\cdot)^n$ and $(\cdot)^{n+1}$ denote the quantity $(\cdot)$ at time t^n and t^{n+1}, respectively. Δt^n is defined as $\Delta t^n = t^{n+1} - t^n$.

3.1 Weak form for $\boldsymbol{v}$

Quasistatic case We solve the rate form of the equilibrium equation to obtain the material velocity field $\boldsymbol{v}$ on the current configuration Ω following the assumed strain formulation of [NPR74]. We define $\delta\bar{\boldsymbol{L}}$ to be

$$\delta\bar{\boldsymbol{L}}(\boldsymbol{x}) := grad\delta\boldsymbol{v}(\boldsymbol{x}) - \frac{1}{3}div\delta\boldsymbol{v}(\boldsymbol{x})\boldsymbol{I} + \frac{1}{3\,|B(\boldsymbol{x})|}\int_{B(\boldsymbol{x})}\boldsymbol{I}\,div\delta\boldsymbol{v}\,dV,$$

where $B(\boldsymbol{x})$ represents the element (in mesh) containing the point $\boldsymbol{x}$ and $|B(\boldsymbol{x})|$ is the volume of the element B. The weak form is then written as

$$\int_\Omega \delta\bar{\boldsymbol{L}} : \left[div\boldsymbol{v}\,\boldsymbol{T} + \dot{\boldsymbol{T}} - \boldsymbol{T}\bar{\boldsymbol{L}}^T\right]\,dV = \int_{\partial\Omega}\delta\boldsymbol{v}\cdot\dot{\boldsymbol{t}}\,dA.$$

where

$$\bar{\boldsymbol{L}}(\boldsymbol{x}) := \boldsymbol{L}(\boldsymbol{x}) - \frac{1}{3}div\,\boldsymbol{v}(\boldsymbol{x})\boldsymbol{I} + \frac{1}{3\,V(\boldsymbol{x})}\int_{B(\boldsymbol{x})}\boldsymbol{I}\,div\,\boldsymbol{v}(\boldsymbol{x})\,dV$$

and $\dot{\boldsymbol{t}}$ is the specified Neumann boundary condition of nominal traction rate based on the current configuration as the reference. Using the evolution equation for $\boldsymbol{W}$ and the identity $\boldsymbol{F}^e\boldsymbol{W} = \boldsymbol{I}$, the material time derivative of $\boldsymbol{T}$ is calculated as

$$\dot{\boldsymbol{T}} = \left(\frac{\partial\boldsymbol{T}}{\partial\boldsymbol{F}^e}\right) : (\boldsymbol{L} - (\boldsymbol{F}^e\boldsymbol{\alpha}) \times \boldsymbol{V} - \boldsymbol{F}^e\boldsymbol{L}^p)\,\boldsymbol{F}^e.$$

Using the expression for $\dot{\boldsymbol{T}}$, the weak form of Eq. (14) is expressed as

$$\int_{\Omega} \delta\,\bar{\boldsymbol{L}} : \left[tr(\bar{\boldsymbol{L}})\boldsymbol{T} - \boldsymbol{T}\bar{\boldsymbol{L}}^T + \frac{\partial \boldsymbol{T}}{\partial \boldsymbol{F}^e} : (\bar{\boldsymbol{L}} \cdot \boldsymbol{F}^e) \right] dV = \underline{\int_{\Omega} \delta\,\bar{\boldsymbol{L}} : \left[\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{F}^e} : ((\boldsymbol{F}^e\boldsymbol{\alpha}) \times \boldsymbol{V})\,\boldsymbol{F}^e \right] dV} + \underline{\int_{\Omega} \delta\,\bar{\boldsymbol{L}} : \left[\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{F}^e} : (\boldsymbol{F}^e\boldsymbol{L}^p\boldsymbol{F}^e) \right] dV} + \int_{\partial\Omega} \delta\bar{\boldsymbol{v}} \cdot \dot{\boldsymbol{t}}\, dA. \tag{15}$$

For a given state of the system ($\boldsymbol{T}^n, \boldsymbol{F}^{e,n}, \boldsymbol{L}^{p,n}, \boldsymbol{\alpha}^n, \boldsymbol{x}^n$, and $\boldsymbol{V}^n$) at time t^n, the weak form generates a system of linear equations which is then solved to get the velocity field $\boldsymbol{v}^n$ on the configuration Ω^n. On part of the boundary where Dirichlet conditions on the velocity are applied, the nodal reaction force rates at time t^n are calculated after solving (15) on the configuration Ω^n. Since such a nodal force rate, viewed as a discrete function of time, corresponds to the evolving current configuration of the body, we simply (discretely) integrate it in time and accumulate the result on the known nodal force at time t^n to obtain the nodal force (on the velocity-Dirichlet-part of the boundary) at time t^{n+1}. On the part of the boundary where Cauchy tractions are specified (including null), nothing needs to be done.

Dynamic case For the dynamic case, the balance of linear momentum equation is directly solved to obtain the velocity on the given configuration. Assuming the stresses and material velocity on the current configuration Ω^n are given, we solve for $\boldsymbol{v}^{n+1}$ using the Forward Euler method as follows:

$$\int_{\Omega^n} \rho\, v_i^{n+1} \delta v_i\, dV = \int_{\Omega^n} \rho\, v_i^n \delta v_i\, dV + \Delta t^n \left(\int_{\partial\Omega^n} t_i \delta v_i\, dA - \int_{\Omega^n} T_{ij} \delta v_{i,j}\, dV \right). \tag{16}$$

3.2 Weak form for $\boldsymbol{\alpha}$

Following [RA05, RA06], we adopt the Galerkin-Least-Squares FEM approach as described in [HFH89] wherein the Galerkin residual is added to a non-negative (may be spatially varying) scalar multiple of the least squares residual. Writing $\boldsymbol{L}^p = \hat{\boldsymbol{L}}^p + \beta\, curl\boldsymbol{\alpha}$, (1a) can be rewritten as

$$tr(\boldsymbol{L})\boldsymbol{\alpha} + \dot{\boldsymbol{\alpha}} - \boldsymbol{\alpha}\boldsymbol{L}^T = -curl\left(\boldsymbol{\alpha} \times \boldsymbol{V} + \hat{\boldsymbol{L}}^p + \beta curl\boldsymbol{\alpha} \right). \tag{17}$$

Using a linearly implicit scheme, the Galerkin-Least-Squares residual for Eq. (17) is written in (18). In (18), no superscript on $\boldsymbol{\alpha}$ refers to $\boldsymbol{\alpha}^{n+1}$. $\boldsymbol{L}$, $\boldsymbol{V}$, and $\hat{\boldsymbol{L}}^p$ are treated as known data. $\partial\Omega_i^n$ and $\partial\Omega_o^n$ represent the inflow and outflow parts of the boundary $\partial\Omega^n$. $\boldsymbol{B}$ is the input dislocation flux $\boldsymbol{\alpha}(\boldsymbol{V}\cdot\boldsymbol{n})$ on $\partial\Omega^n$. Ω_e^n denotes the element interiors. c is the non-negative (possibly spatially varying) scalar that takes the value 1 in the convection dominated regions and is equal to the grid Péclet number in diffusion dominated regions. Since we take l (see Eqs. (5) and (7)) to be very small, we choose $c = 1$ for MFDM calculations, unless stated otherwise.

$$
\begin{aligned}
R = & \int_{\Omega^n} \delta\alpha_{ij} \left(\Delta t^n \, L_{pp}\alpha_{ij} - \Delta t^n \, \alpha_{ip} L_{jp} \right) \, dV + \int_{\Omega^n} \delta\alpha_{ij} \left(\alpha_{ij} - \alpha_{ij}^n \right) \, dV \\
& + \Delta t^n \int_{\Omega^n} \varepsilon_{jqp} \, \varepsilon_{jab} \alpha_{ia} V_b \delta\alpha_{ip,q} \, dV \\
& + \Delta t^n \int_{\Omega^n} \hat{L}_{ij}^p \varepsilon_{jqp} \delta\alpha_{ip,q} \, dV + \Delta t^n \int_{\Omega^n} \beta \varepsilon_{jab} \alpha_{ib,a} \varepsilon_{jqp} \delta\alpha_{ip,q} \, dV \\
& + \Delta t^n \int_{\partial\Omega_i^n} B_{ij} \delta\alpha_{ij} \, dA + \Delta t^n \int_{\partial\Omega_o^n} \alpha_{ij}^n V_p n_p \delta\alpha_{ij} \, dA - \Delta t^n \int_{\partial\Omega^n} \alpha_{iq} V_j n_q \delta\alpha_{ij} \, dA \\
& - \Delta t^n \int_{\partial\Omega^n} \varepsilon_{jpq} \hat{L}_{ip}^p n_q \delta\alpha_{ij} \, dA - \Delta t^n \int_{\partial\Omega^n} \beta \varepsilon_{jpq} \varepsilon_{pba} \alpha_{ia,b} n_q \delta\alpha_{ij} \, dA \\
& + c \left[\int_{\Omega_e^n} A_{ri} \delta\alpha_{ri} \, dV + \Delta t^n \int_{\Omega_e^n} L_{pp} A_{ri} \delta\alpha_{ri} \, dV - \Delta t^n \int_{\Omega_e^n} A_{ri} \delta\alpha_{rp} L_{ip} \, dV \right. \\
& + \Delta t^n \int_{\Omega_e^n} A_{ri} \left(\delta\alpha_{ri,q} V_q - \delta\alpha_{rq,q} V_i + \delta\alpha_{ri} V_{q,q} - \delta\alpha_{rq} V_{i,q} \right) \, dV \\
& \left. + \Delta t^n \int_{\Omega_e^n} A_{ri} (\beta_{,p} \delta\alpha_{rp,i} + \beta \delta\alpha_{rp,ip} - \beta_{,p} \delta\alpha_{ri,p} - \beta \delta\alpha_{ri,pp}) \, dV \right],
\end{aligned}
\tag{18}
$$

where

$$
\begin{aligned}
A_{ri} = \alpha_{ri} - \alpha_{ri}^n + \Delta t^n \Big[& \alpha_{ri}^n L_{pp} - \alpha_{rp}^n L_{ip} + \alpha_{ri,q}^n V_q - \alpha_{rq,q}^n V_i + \alpha_{ri}^n V_{q,q} - \alpha_{rq}^n V_{i,q} + \varepsilon_{ipq} \hat{L}_{rq,p}^p + \\
& + \beta_{,p} \alpha_{rp,i}^n + \beta \alpha_{rp,ip}^n - \beta_{,p} \alpha_{ri,p}^n - \beta \alpha_{ri,pp}^n \Big] .
\end{aligned}
$$

3.3 Evolution of $\boldsymbol{f}$

The evolution equation (1c) for $\boldsymbol{f}$ is solved on the current configuration at each time step with the natural b.c.s imposed on the external boundary. Letting $\boldsymbol{Y} = (\boldsymbol{\alpha} \times \boldsymbol{V} + \boldsymbol{L}^p - \dot{\boldsymbol{\chi}} - \boldsymbol{\chi}\boldsymbol{L})$ and using a forward Euler scheme to update $\boldsymbol{f}$, the weak form of (1c) is

$$
\int_{\Omega^n} grad \, \boldsymbol{f}^{n+1} : grad \, \delta\boldsymbol{f} \, dV = \Delta t^n \int_{\Omega^n} \boldsymbol{Y}^n : grad \, \delta\boldsymbol{f} \, dV + \int_{\Omega^n} grad \, \boldsymbol{f}^n : grad \, \delta\boldsymbol{f} \, dV. \tag{19}
$$

3.4 Weak form for $\boldsymbol{\chi}$

For a given dislocation density $\boldsymbol{\alpha}$ and a configuration of the body Ω, $\boldsymbol{\chi}$ is evaluated by solving the system (1b) along with the Dirichlet boundary conditions $\boldsymbol{\chi} \cdot \boldsymbol{n} = \boldsymbol{0}$. We use the Least-Squares finite element method to solve for $\boldsymbol{\chi}$ from the *div-curl* system (1b). The weak form, given below, can be easily solved to obtain $\boldsymbol{\chi}$ on a given configuration Ω for a given dislocation density.

$$
\int_{\Omega} e_{ijk} \delta\chi_{rk,j} \left(e_{imn} \chi_{rn,m} + \alpha_{ri} \right) \, dV + \int_{\Omega} \delta\chi_{ij,j} \chi_{im,m} \, dV = 0. \tag{20}
$$

3.5 Adjusting $\boldsymbol{f}$ from equilibrium equation

We use the Newton-Raphson scheme to solve for $\boldsymbol{f}$ at large deformation as the governing equation $div[\boldsymbol{T}(\boldsymbol{f}, \boldsymbol{\chi})] = \boldsymbol{0}$ is nonlinear in $\boldsymbol{f}$. Following the scheme outlined in [Pur09], we write the residual from the variational statement for $(1d)_1$

$$R(\boldsymbol{f}) = \int_{\partial\Omega} t_i \delta f_i \, dA - \int_{\Omega} T_{ij} \delta f_{i,j} \, dV. \tag{21}$$

The guess for this Newton-Raphson solve is crucial for success in solving for $\boldsymbol{f}$. We denote this guess as $\boldsymbol{f}_0$ and it is determined, following [ZAP18], as follows:
1. For ECDD solves ($t = 0$), $\boldsymbol{f}_0$ is obtained by solving the equilibrium equation on the current configuration by assuming small deformation.

2. At any other time ($t > 0$), $\boldsymbol{f}^{n+1}$ obtained by solving the evolution equation (19) serves as the guess $\boldsymbol{f}_0$ for the Newton-Raphson based scheme.

The linear system is then iteratively solved until the norm of the discrete residual $|R_a^A|$ is less than a tolerance of $10^{-12}\, g_0\, h^2$ (in 2-d), where h denotes the length of the smallest edge of an element in the finite element mesh.

4 Algorithms

We choose a combination of explicit-implicit schemes to evolve the coupled system (Eqs. (15), (20), (17), (19)) in time. An efficient time stepping criteria based on plastic relaxation, and purely elastic and 'yield strain' related physical model parameters has been developed.

The following notation is used for the description of the algorithm:

1. $(\cdot)^n$ means a quantity at time t^n. $\boldsymbol{x}^n$ represents the coordinates of the finite element mesh on the configuration Ω^n.

2. At any integration point q, the following state variables are stored at any given time t^n: material strength g^n, elastic distortion tensor $\boldsymbol{F}^{en}$, Cauchy stress $\boldsymbol{T}^n$, dislocation velocity $\boldsymbol{V}^n$, slip distortion rate $\boldsymbol{L}^{pn}$. We will collectively refer to them as PH^n (short for point history) of integration points.

3. Δt^n is defined as $t^{n+1} - t^n$. To evaluate Δt^n we first calculate the following variables at each time-step

$$\Delta t_1 = \frac{\xi\, h}{\max(|\boldsymbol{V}^n|)} \quad ; \quad \Delta t_2 = \frac{.002}{\max(|\boldsymbol{F}^{en}\boldsymbol{\alpha}^n \times \boldsymbol{V}^n|) + \max(\hat{\gamma}_{sd}^n)}$$

$$\Delta t_3 = \frac{\xi\, g_0}{E\, \max(|\boldsymbol{L}^n|)} \quad ; \quad \Delta t_4 = \frac{\xi\, h}{v_s}$$

where $\max(\cdot)$ denotes the maximum of the quantity $(\cdot)$ over all integration points in the domain, h denotes the length of the smallest edge of an element in the finite element mesh, v_s is the shear wave speed of the material, and ξ is a scalar currently chosen to be 0.1.

Δt^n is then given as

$$\Delta t^n = \begin{cases} \min\left(\Delta t_1, \Delta t_2, \Delta t_3\right) & \text{Quasistatic case} \\ \min\left(\Delta t_1, \Delta t_2, \Delta t_3, \Delta t_4\right) & \text{Dynamic case} \end{cases} \tag{22}$$

Given: material properties, initial conditions, boundary conditions, and applied loading conditions.
Step 1: Find the initial stress field on the body in 'as-received' configuration - ECDD solve.
Step 2: Evolution of the system: Assume that the state at time t^n is known: $\boldsymbol{x}^n$, $\boldsymbol{\alpha}^n$, $\boldsymbol{f}^n$, $\boldsymbol{\chi}^n$, $\dot{\boldsymbol{\chi}}^n$, $\boldsymbol{V}^n$, $\boldsymbol{L}^p$, Δt^n, PH^n To get the state at time step t^{n+1} the following is done: 1. The rate form of the equilibrium equation (14) is solved on Ω^n to get the material velocity $\boldsymbol{v}^n$ using Eq. (15). 2. Weak form of $\boldsymbol{\alpha}$ evolution equation (18) is solved on Ω^n to obtain $\boldsymbol{\alpha}^{n+1}$ on Ω^{n+1}. 3. The configuration of the body is discretely updated i.e. $\boldsymbol{x}^{n+1} = \boldsymbol{x}^n + \boldsymbol{v}^n \Delta t^n$. 4. $\boldsymbol{\chi}^{n+1}$ on Ω^{n+1} is obtained by solving Eq. (20) on Ω^{n+1}. 5. $\boldsymbol{f}^{n+1}$ on Ω^{n+1} is obtained by doing one of the following: a Solve Eq. (19) on Ω^n to obtain $\boldsymbol{f}^{n+1}$. b. Solve equilibrium equation (1d) in alternate increments to adjust $\boldsymbol{f}^{n+1}$ on Ω^{n+1} as shown in Eq. (21). $\boldsymbol{f}^{n+1}$ obtained by solving Eq. (19) serves as the initial guess for the Newton Raphson scheme. 6. $\dot{\boldsymbol{\chi}}^{n+1}$ is calculated as follows: $\dot{\boldsymbol{\chi}}^{n+1} = \dfrac{\boldsymbol{\chi}^{n+1} - \boldsymbol{\chi}^n}{\Delta t^n}$. 7. PH^{n+1} is updated on the configuration Ω^{n+1}.

Table 6: Quasi-static MFDM algorithm.

The algorithms for the quasistatic and dynamic cases are shown in Tables 6 and 7, respectively.

5 Parallel computation complexity and justification for requested service units

- *Runs are to be conducted* For each individual problem, we mention the parameters to be studied and an estimated number of runs required to successfully study that problem. The mentioned problems use the same algorithm and numerical framework, so there is no difference in the computational complexity of iterations even when the parameters are changed.
- *Access to other resources*: We have a total of 4 machines in our group - 3 machines in our group with 16 cores each and one machine with 80 cores. These machines are mainly used for debugging the the code and post-processing the results. The access to above mentioned resources are already taken into consideration while submitting this renewal request.

In this renewal, we request an allocation of 415,000 service units on Bridges-2 and 30 TB of storage on Bridges-2 file system, Ocean. The allocations are estimated based on the computational complexity of the numerical algorithms of Mesoscale Field Dislocation Mechanics (MFDM), and an approximation of number of SUs required to simulate problems listed below for around 512K elements in the mesh. With the requested service units, MFDM will be applied to model the following mesoscopic scale problems in plasticity (We did make little progress on these problems during our last allocation):

1. *Dislocation Avalanche mechanism in High Entropy Alloys:* We plan to study the dislocation avalanche formation in the compressed nanopillars made of of high entropy alloy, $Al_{0.1}CrCoFeNi$. Recent experimental observations [HSY+18] show that the avalanche starts with dislocation accumulation and formation of the deformation bands along with sudden stress drops in the stress-strain curves of the sample. Using the constitutive assumptions for $\boldsymbol{V}$ and $\boldsymbol{L}^p$ from crystal plasticity in our

Given: material properties, initial conditions, boundary conditions, and applied loading conditions.
Step 1: ECDD solve as outlined in the Table 6 is done on the initial configuration, i.e. current configuration at $t = 0$, to determine $\boldsymbol{f}$, $\boldsymbol{\chi}$, and $\boldsymbol{T}$ at $t = 0$.
Step 2: Evolution of the system: Assume that $\boldsymbol{v}^{n-1}$ and the state at time t^n is known: $\boldsymbol{x}^n$, $\boldsymbol{\alpha}^n$, $\boldsymbol{f}^n$, $\boldsymbol{\chi}^n$, $\dot{\boldsymbol{\chi}}^n$, $\boldsymbol{V}^n$, $\boldsymbol{L}^p$, Δt^n, PH^n To get the state at time step t^{n+1} the following is done: 1. The balance of linear momentum Eq. (14) is solved on Ω^n to get the material velocity $\boldsymbol{v}^n$ using Eq. (16). 2. Weak form of $\boldsymbol{\alpha}$ evolution equation (18) is solved on Ω^n to obtain $\boldsymbol{\alpha}^{n+1}$ on Ω^{n+1}. 3. $\boldsymbol{f}^{n+1}$ on Ω^{n+1} is obtained by solving Eq. (19). 4. The configuration of the body is discretely updated i.e. $\boldsymbol{x}^{n+1} = \boldsymbol{x}^n + \boldsymbol{v}^n \, \Delta t^n$. 5. $\boldsymbol{\chi}^{n+1}$ on Ω^{n+1} is obtained by solving Eq. (20) on Ω^{n+1}. 6. $\dot{\boldsymbol{\chi}}^{n+1}$ is calculated as follows: $\dot{\boldsymbol{\chi}}^{n+1} = \dfrac{\boldsymbol{\chi}^{n+1} - \boldsymbol{\chi}^n}{\Delta t^n}$. 7. PH^{n+1} is updated on the configuration Ω^{n+1}.

Table 7: Dynamic (with inertia) MFDM algorithm.

framework, and mirroring the experimentally used setup for compression, our study will provide critical insights into the deformation of high entropy alloys. Since it takes around $30K$ increments to reach upto 30% strain, a single successful run will require around $11K$ CPU hours (as per the calculation shown in scaling document). To study the effects of latent hardening, material saturation strength, and prescribed initial dislocation distribution, we plan to do around 15 runs (5 runs for each parameter) for these simulations. **Request**: 165K SUs for 15 runs.

2. *Response of Polycrystalline aggregates*: Motivated by the experimental observations [HH95] and [HH97], we plan to study the response of polycrystalline aggregates in the framework on MFDM. At large strains, significant changes in the microstructure and the texture are observed experimentally wherein the microstructure evolves into a lamellar structure with boundaries of small to medium misorientation angles mixed with high angle boundaries - which we plan to investigate using our developed framework for MFDM, This problem requires refined mesh at the grain boundaries and therefore will need higher resources (≈ 1.5 times) than other problems. We plan to study the effects of material strength, plastically constrained and unconstrained boundary conditions, and different domain sizes which will require 15 runs. **Request**: 250K SUs for 15 runs. *Note*: We planned to work on this problem in our last allocation but we worked on a different problem (mentioned in progress report).

All the estimations are based on the scaling arguments presented in the code scaling document, i.e., performing a productive MFDM simulation with 512K elements in $3d$ upto 30K increments which results in an approximate 11K Core·hours for one simulation. We request a total of $415,000$ CPU·hours on PSC Bridges-2 Regular Memory (RM) nodes for running the the above mentioned simulations. After a fixed iteration count, each processor generates an output file at every time increment that corresponds to the locally owned elements in the finite element mesh. The code also generates restart/checkpoint files after a few hundred iterations, so that the simulation can be restarted in case of an unexpected failure. From the previous experience of file sizes generated during the runs, we request 30 TB of storage on Bridges-2 for storing all the data generated during the runs and accommodating the useful data from the previous allocations.

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