Use of spherical harmonics for dislocation dynamics in anisotropic elastic media

To cite this article: S Aubry and A Arsenlis 2013 Modelling Simul. Mater. Sci. Eng. 21 065013

View the article online for updates and enhancements.
Use of spherical harmonics for dislocation dynamics in anisotropic elastic media

S Aubry and A Arsenlis

Lawrence Livermore National Laboratory, Livermore, CA, USA

Received 14 January 2013, in final form 6 June 2013
Published 8 August 2013
Online at stacks.iop.org/MSMSE/21/065013

Abstract
Large-scale dislocation dynamics simulations usually involve several millions of interacting dislocation segments. The stress at a point and interaction force between two segments need to be computed many times during simulations. We evaluate the cost versus accuracy of using spherical harmonics series to approximate the anisotropic elastic Green’s function in calculating stresses and forces between segments. The stress at a point is obtained by analytically integrating the spherical harmonics series once and the forces by integrating it analytically twice. We analyze the convergence and cost of using this approach and describe the elements of a fast implementation. We find that the cost of the force and stress calculations grows quadratically with the accuracy for a fixed anisotropy ratio.

1. Introduction

Dislocation dynamics (DD) simulations often assume isotropic elasticity to compute stresses at points in the simulation volume and forces between dislocations. Anisotropic elasticity has been used to compute dislocation reactions and dynamics for small dislocation ensembles such as a dislocation loop, a Frank–Read source and two straight, interacting dislocations [1–6]. For large, dense dislocation ensembles, anisotropic elasticity is rarely used due to its perceived computational cost. Most large-scale simulations have resorted to using isotropic elastic approximations that are less computationally intensive.

Qualitative differences have been observed between isotropic and anisotropic media in the literature. For high anisotropy, such as for α-iron at high temperatures with an anisotropy ratio of $A \approx 7.5$, it has been shown analytically [1], numerically [2] and experimentally [3] that prismatic and glide loops form sharp corners. It was also observed that the critical stress to bow out a Frank–Read source changes with anisotropy [4]. These observations suggest that dislocation mechanisms can be significantly altered when full elastic anisotropy is considered. For a quantification of the error made using isotropic elasticity, Rhee et al [5] suggested an error as high as 15% for some components of the stress tensor in a hexagonal dislocation loop in molybdenum with an anisotropy ratio of $A = 0.775$. Also, Han et al [7] concluded that the
stress–strain behavior of copper with an anisotropy ratio of \( A = 3.21 \) cannot be reproduced using isotropic approximations.

However, some studies have also claimed that the mechanical response of polycrystalline copper might not be very sensitive to anisotropy effects [8]. This low sensitivity is reported to be caused by the averaging over many grains. In general, it remains unclear when it is acceptable to use the isotropic approximation with Reuss or Voigt averaged constants for an elastically anisotropic crystal. It is unclear whether there is a critical level of elastic anisotropy that requires the use of a full anisotropic formalism, and it is unclear whether the errors associated with using an isotropic approximation for a generally anisotropic medium can be bounded.

The main reason anisotropic elasticity is not used in large-scale DD simulations is its perceived cost. It has been shown that using the Willis–Steeds or the Brown formula [9] to compute interactions between dislocations in anisotropic elasticity can be orders of magnitude slower than the equivalent calculation in isotropic elasticity. The exact cost depends on the way forces between interacting dislocation segments are computed as well as the distance separating the segments [5, 7, 10]. The main difficulty in using anisotropic elasticity is that an analytical form of the anisotropic Green’s function does not exist. The analytical form of the Green’s function in isotropic elasticity has led to analytical expressions for the stress at a point and the force between two interacting segments [11]. The use of analytical forms enables a fast calculation of stresses and forces compared with numerical integration. Since an analytical definition of the Green’s function is lacking in anisotropic elasticity, several attempts have been made to describe it efficiently. For instance, Rhee et al [5] defined look-up tables to determine the angular part of the Green’s function and its derivative. Unfortunately, these methods remain expensive and have seen a limited use in DD. They still require numerical integration of forces, and the accuracy and cost vary with relative distance between segments: the closer the interacting dislocation segments, the more the Gauss quadrature points that are necessary to compute the forces between interacting pairs of segments accurately.

In this paper, we propose a fast implementation of dislocation interactions in anisotropic media that is practical for large-scale simulations. The method is illustrated for the classical Volterra dislocation, using the singular theory recounted in Hirth and Lothe [9]. The key is to represent the Green’s function with a spherical harmonics series. Mura and Kinoshita proposed this representation in 1971 [12]. In [12], Mura describes how the Green’s function and its derivatives can be expanded in spherical harmonics series. The novelty is to observe that such a decomposition allows the single line integral involved in the definition of the stress at a point and the double line integral involved in the calculation of the forces to be expressed analytically once the coefficients of the series have been set. This alleviates the need for numerical integration and drastically decreases the cost of stress and force evaluations.

Section 2 describes the expansion of the derivative of the Green’s function into a spherical harmonics series and the integration procedure of that series leading to series expressions for the stress at a point due to a dislocation segment and the force between interacting segments. Section 3 shows how the integration of the spherical harmonics series can be computed in an efficient manner. Section 4 shows the numerical results for cost and accuracy of the proposed method. The last section compares our method with existing methods.

2. Stress and interaction forces in anisotropic elasticity

In DD simulations, dislocations are discretized into nodes connected by segments. The stress at a point due to a dislocation segment and the interaction force between a pair of segments can be defined using linear elasticity.
Figure 1. Notation for two interacting segments: dislocation segment \([x_1, x_2]\) with line direction \(t'\), length \(L'\) and Burgers vector \(b'\) and segment \([x_3, x_4]\) with line direction \(t\), Burgers vector \(b\) and length \(L\). If \(x\) is a point on \([x_3, x_4]\) and \(x'\) a point on segment \([x_1, x_2]\), then \(R = x - x'\).

In a linear elastic domain, the stress at \(x\) due to a dislocation loop \(C\) with elastic stiffness tensor \(C_{ijkl}\) is given by Mura et al's formula [9]

\[
\sigma_{js}(x) = \epsilon_{gij} C_{jxq} C_{pqwx} b_w \int_{C} \frac{\partial G_{vp}}{\partial x_q} (x - x') \, dx'_v
\]

(1)

where \(\partial G_{vp}/\partial x_q\) is the first derivative of the Green’s function, defined in more detail below, \(b'\) is the Burgers vector of the dislocation loop and \(\epsilon\) is the permutation tensor. The stress is determined uniquely when the integral is evaluated on a closed loop. This loop can be decomposed over a sum of straight segments to form a discretized polygonal loop.

In the DD code ParaDiS [11], forces are defined at the end nodes of dislocation segments. There are a couple of equivalent ways to compute the force on a node of a discretized dislocation configuration. The force can be found as the minus derivative of the total energy with respect to the node position. Alternatively, the force on a node can be obtained using the virtual force argument, i.e. by computing appropriate line integrals of the Peach–Koehler force over the segments connected to the node. Consider two segments \([x_1, x_2]\) and \([x_3, x_4]\) with Burgers vectors \(b'\) and \(b\) and lengths \(L'\) and \(L\), respectively; see figure 1 for notation. The contribution from segment \([x_1, x_2]\) to the force on node \(x_4\) is equal to the work of the Peach–Koehler force as the segment sweeps over a triangular-shaped area due to a virtual displacement of node \(x_4\) [11], i.e.

\[
F^4 = \int_{x_4}^{x_3} N(x) \sigma_{12}(x) \cdot b \times dx
\]

where \(N\) is the shape function \(N(x) = \frac{|x - x_4|}{|x - x_3|}\), \(x\) is a point on segment \([x_3, x_4]\) and is defined such that it equals one when \(x = x_4\) and zero when \(x = x_3\).

When we evaluate the stress on a finite segment \([x_1, x_2]\), the force becomes a double line integral over the two dislocation segments,

\[
F_i^4 = \epsilon_{ij} \epsilon_{gij} C_{jxq} C_{pdun} b_p b_n \int_{x_1}^{x_2} \int_{x_3}^{x_4} \frac{\partial G_{vp}}{\partial x_d} (R) \frac{|x - x_3|}{L} \, dx_d \, dx'_v
\]

(2)

where \(R = x - x'\) is the distance between two points \(x\) and \(x'\) belonging to the two dislocation segments \([x_3, x_4]\) and \([x_1, x_2]\), respectively.

This latter definition of the force at a node, equation (2), is convenient for force calculations as it explicitly gives the interaction force on the end nodes of the dislocation segments. Arsenlis et al [11] showed that in isotropic elasticity, the force defined in equation (2) can be computed analytically thereby preventing expensive numerical integration.
2.1. Definition of the Green’s function and its derivative

The stress and the interacting force between dislocations are defined through the Green’s function. The Green’s function \( G_{kp}(x - x') \) is defined as the displacement in the \( x_k \)-direction at point \( x \) in response to a unit point force in the \( x_p \)-direction applied at point \( x' \). It is given explicitly in isotropic elasticity but not in anisotropic elasticity. The Green’s function in anisotropic elasticity has been described in detail by Bacon et al [13] as

\[
G_{kp} = \frac{1}{4\pi^2 R^2} \int_0^\pi M_{kp}^{-1}(\xi) \, d\psi
\]

where \( M_{kp}^{-1}(\xi) \) is defined as

\[
M_{kp}^{-1}(\xi) = \frac{\epsilon_{kms}\epsilon_{prw}(\xi\xi)_{sr}(\xi\xi)_{mw}}{2\epsilon_{ipa}(\xi\xi)_{ij}(\xi\xi)_{2j}(\xi\xi)_{3i}}
\]

where the notation \((\xi\xi)_{ij} = \xi_i \xi_j\) is used. The matrix \( M^{-1} \) is a quotient of polynomials of the order of four in the numerator and six in the denominator. \( R \) is the norm of \( \mathbf{T} \) and \( \mathbf{T} = \mathbf{R}/R \) its direction. The vector \( \mathbf{\xi}(\psi) \) is a unit vector for which \( \mathbf{\xi} \cdot \mathbf{T} = 0 \) and varies in the plane formed by \((\mathbf{\hat{e}}_x, \mathbf{\hat{e}}_y)\) with an angle \( \psi \). Vectors \( \mathbf{\hat{e}}_x \) and \( \mathbf{\hat{e}}_y \) are two arbitrary unit vectors defined in the plane orthogonal to \( \mathbf{T} \); see figure 2 for notation. More details can be found in [13, 14]. A closed form analytical expression for the Green’s function’s integral does not exist.

The derivative of the Green’s function is given in Barnett [14] as

\[
\frac{\partial G_{kp}}{\partial x_q} = \frac{1}{4\pi^2 R^2} \int_0^\pi \left(-T_q M_{kp}^{-1} + \xi_q N_{kp}\right) \, d\psi
\]

where

\[
N_{kp} = C_{jrwu} M_{kj}^{-1} M_{wp}^{-1} (\xi_r T_w + \xi_u T_v).
\]

As defined, the derivative of the Green’s function is a product of a part depending only on \( 1/R^2 \) and an angular part \( g \) depending only on the direction \( \mathbf{T} \)

\[
g_{vpd}(\mathbf{T}) = g_{vpd}(\theta, \phi) = \int_0^\pi \left(-T_d M_{vp}^{-1} + \xi_d N_{vp}\right) \, d\psi
\]

where \((\theta, \phi)\) are the spherical coordinates of \( \mathbf{T} \), so that the derivative of the Green’s function is

\[
\frac{\partial G_{vp}}{\partial x_d}(\mathbf{R}) = \frac{g_{vpd}(\mathbf{T})}{4\pi^2 R^2}.
\]

There exists no analytical expression for \( g_{vpd} \); however, the function \( g_{vpd}(\mathbf{T}) \) is suitable for decomposition in spherical harmonics.
2.2. Decomposition in spherical harmonics

A continuous function $g$ on the unit sphere can be expanded in a series of spherical harmonics

$$g(T) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} g_l^m Y_l^m(T)$$

which uniformly converges on the unit sphere [12].

The expansion coefficients $g_l^m$ are independent of $T(\theta, \phi)$ and are defined as

$$g_l^m = \int_{0}^{2\pi} \int_{0}^{\pi} g(\theta, \phi) Y_l^m(\theta, \phi) \sin \theta \, d\theta \, d\phi.$$

(6)

The spherical harmonics $Y_l^m$ are defined as the complex functions

$$Y_l^m(\theta, \phi) = M_l^m P_l^m(\cos \theta) e^{im\phi}$$

where $M_l^m = \sqrt{(2l+1)/(4\pi)} P_l^m$ and $P_l^m$ are the associated Legendre polynomials [15]. For any $m \in [-l, l]$, the spherical harmonics can be written explicitly as

$$Y_l^m(T) = (-1)^m M_l^m f_m(x, y) \frac{(2l - 2k)!}{2(l-k)k!(l-2k-[m]!)} (-1)^k z^{-[m]-2k}$$

(7)

with

$$f_m(x, y) = \begin{cases} (x + iy)^m & \text{if } m \geq 0 \\ (x - iy)^{-m} & \text{if } m < 0 \end{cases}.$$

All the factorials in equation (7) can be expressed using the binomial coefficients and rewritten in the form

$$Y_l^m(T(x, y, z)) = f_m(x, y) \sum_{k=0}^{[l-[m]/2]} \tilde{Q}_l^m(k) z^{-[m]-2k}$$

(8)

where

$$\tilde{Q}_l^m(k) = \frac{(-1)^{m+k} m!}{4\pi^2} \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} \binom{l}{k} \binom{2l-2k}{l} \binom{l-2k}{m}.$$

(9)

The function $g$ can be defined in terms of equations (8) and (9) as

$$g(x, y, z) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} 2^m \binom{l}{l} g_l^m \sum_{k=0}^{[l-[m]/2]} \tilde{Q}_l^m(k) z^{-m-2k}$$

(10)
where we have noted $\Re(x)$ the real part of $x$ and $Q^0_m(k) = \tilde{Q}^0_m(k)$ when $m = 0$ and $Q^m_m(k) = 2 \tilde{Q}^m_m(k)$, when $m > 0$.

Applying the spherical harmonics series expansion to the angular part of the derivative on the Green’s function and defining $\sigma_{js}(x)$ as a function of the derivative of the Green’s function, they can also be expanded in powers of $1/R$: $l$ means that in the expansion in spherical harmonics, the non-zero terms correspond to odd powers of $1/R$. This property means that in the expansion in spherical harmonics, the non-zero terms correspond to odd powers of $1/R$. For isotropic elasticity, the expansion in spherical harmonics is exact and only requires a truncated expansion up to $q = 1$.

2.3. Stress and forces in anisotropic elasticity in terms of spherical harmonics

Since the stress at a point, equation (1), and the force on an end node, equation (2) can be written as a function of the derivative of the Green’ function, they can also be expanded in series using equation (11):

$$\sigma_{js}(x) = \epsilon_{ij} r C_{jsvxg} C_{pdwnb'_w} \sum_{q=0}^{2q+1} \sum_{m=0}^{[l-m]/2} \Re \left( S_{vpd}^{qm} \left( \frac{(R \cdot e_{12})^m (R \cdot e_3)^{2q+1-m}}{R^{2q+3}} \right) \right) \int_{x_1}^{x_2} dx'_i$$

where $S_{vpd}^{qm}$ is a sum of products composed of $Q^m_l(k)$ and $g^m_{l,pd}$.

The Green’s function and its derivative depend only on odd powers of $1/R$. This property means that in the expansion in spherical harmonics, the non-zero terms correspond to odd powers of $1/R$. For isotropic elasticity, the expansion in spherical harmonics is exact and only requires a truncated expansion up to $q = 1$.

$$\frac{\partial G_{ip}(R)}{\partial x_d}(R) = \sum_{q=0}^{2q+1} \sum_{m=0}^{[l-m]/2} \Re \left( Q^m_l(k) g^m_{l,pd} \left( \frac{(R \cdot e_{12})^m (R \cdot e_3)^{2q+1-m}}{R^{2q+3}} \right) \right)$$

These equations for the stress and the force reveal single and double integrals over the dislocation segments. The advantage of writing the stress and the force using expansion in spherical harmonics series is the possibility of efficiently deriving these integrals analytically via recurrence. The calculations of the single line integral

$$J_{ijp}(R) = \int \frac{(R \cdot e_3)^i (R \cdot e_{12})^j}{R^p} ds$$

and the double line integral

$$H_{ijp}(R) = \int \int \frac{(R \cdot e_3)^i (R \cdot e_{12})^j}{R^p} dr ds$$

using recurrence relations are given in the appendix. Following the definition of the stress and the force, the powers $i$, $j$ and $p$ are linked by the relation $i + j = p - 2$ which limits the number of integrals to compute. Furthermore, $p$ is odd and $p \geq 3$.

Section B.1 in the appendix gives the recurrence relations for the force in the case of two non-parallel, non-intersecting segments. Section B.2 in the appendix gives the...
recurrence relations in the case of two parallel, non-intersecting segments. Section B.3 in the appendix gives the recurrence relations in the case of two collinear, non-intersecting segments. Appendix A gives the recurrence relations for the stress at a point whether or not the point is collinear to the segment.

3. Implementation of anisotropic elastic stress and force

Several elements in the force and stress formula can be precomputed independently of the dislocation segments for faster calculation.

The product $S_{vpd}^{am}$ is a function of expansion coefficients $g_{vpd}^{lm}$. It does not depend on the exact geometry of the interacting pair of segments and can be precomputed once at the beginning of the simulation.

The $3 \times 3 \times 3 \times 3$ stiffness tensor $C_{ijkl}$ is often written in contracted matrix notation $C_{\alpha \beta}$, a $6 \times 6$ matrix, to take advantage of symmetry in the strain definition. For instance, a $3 \times 3$ tensor $A$ can be written as a six-dimensional vector

$$A = \begin{pmatrix} A_{11} \\ A_{22} \\ A_{33} \\ A_{12} + A_{21} \\ A_{23} + A_{32} \\ A_{31} + A_{13} \\ A_{31} + A_{13} \end{pmatrix}$$

and we can define an operator $\alpha$ such that $A_\alpha = o_{ij}[A_{ij}]$ by the transformation defined in equations (16) where $\alpha$ varies in $\{1, 6\}$ and $(i, j)$ in $\{1, 3\}$.

Using symmetries, the series expansion of the stress, equation (12), can be simplified. The $3 \times 3$ matrix $I_{vpd}$ defined as

$$I_{vpd} = \sum_{q=0}^{\infty} \sum_{m=0}^{2q+1} \Re \left( S_{vpd}^{am} \int_0^L \frac{(R \cdot e_{12})^m (R \cdot e_3)^{2q+1-m}}{R^{2q+3}} \, d\xi' \right)$$

can be contracted into a $3 \times 6$ matrix, $I_{\alpha \beta} = o_{\alpha \beta}^{pd}[I_{vpd}]$. In the definition of the integral, the change of variable $x' = (1 - \xi')x_1 + \frac{1}{2}x_2$ has been made.

The $3 \times 3 \times 3$ matrix $B'$ defined as

$$B'_{pdg} = \sum_{w,n,r} C_{pdwn} \epsilon_{neg} b'_{w r}$$

can also be contracted as a $6 \times 3$ matrix noted $B'_{\alpha \beta \gamma} = o_{\alpha \beta \gamma}^{pd}[B'_{pdg}]$. Using the definitions of $I$ and $B'$, the stress becomes

$$\sigma_{js}(x) = C_{jswg} B'_{pdg} I_{vpd}$$

and the contracted form of the stress at a point $\sigma_{j}(x)$ from equation (12) can be written as

$$\sigma_{j}(x) = C_{j\alpha \gamma} o_{\alpha \gamma}^{pd} [I B']$$

Similarly, the expression, equation (13), for the force can also be simplified. The $3 \times 3 \times 3$ matrix

$$O_{vpd} = \sum_{q=0}^{\infty} \sum_{m=0}^{2q+1} \Re \left( S_{vpd}^{am} \int_0^L \int_0^L \frac{(R \cdot e_{12})^m (R \cdot e_3)^{2q+1-m}}{R^{2q+3}} \frac{L}{L} \, d\xi \, d\xi' \right)$$
can be contracted into a $3 \times 6$ matrix, $O_{\alpha\beta} = o_{\alpha\beta}^{\nu \varphi}[O_{\nu \varphi d}]$. In the definition of the integrals, the changes of variable $x = (1 - \xi) x_3 + \frac{\xi}{2} x_4$ and $x' = (1 - \xi') x_1 + \frac{\xi'}{2} x_2$ have been made. The $3 \times 3 \times 3$ matrix $A$ whose components are

$$A_{ivg} = \sum_{j,s,o} C_{jvsg} \epsilon_{ijos} b_j t_o$$

can also be contracted as a $3 \times 6$ matrix $A_{i\beta \nu} = o_{\nu \varphi}^{\nu \varphi}[A_{ivg}]$.

Using the three matrices $A$, $B'$ and $O$, the force becomes

$$F_i^4 = A_{ivg} B_p \nu d O_{\nu \varphi d}$$

and the contracted form of the force from equation (13) can be written as

$$F_i^4 = A_{i\beta} o_{\nu \varphi}^{\nu \varphi}[O B'].$$ 

4. Numerical results

The expansion of the force in spherical harmonics series in equation (13) depends on expansion coefficients $g_{l \nu \varphi d}$, defined in equation (6) and on the integrals $H_{ijkl}$, defined in equation (15). The expansion coefficients $g_{l \nu \varphi d}$ are defined as a double integral over angles $(\theta, \phi)$ of the function $g(\theta, \phi)$; equation (6). For a fixed couple of angles $(\theta, \phi)$ or direction $T$, the function $g(T)$ is also defined as an integral over an angle $\psi$, as shown by equation (4).

For a given direction $T$, evaluating the function $g$ involves a numerical integration over $\psi \in [0, \pi]$. The number of angles $\psi$ needed to describe this integral is shown in figure 3(a). The error in calculating $g$ at a point on the sphere varies as a function of the number of angles chosen to discretize the integral. Approximately 100 angles are sufficient to obtain machine precision accuracy for a material with an anisotropy less than 8.

The expansion coefficients $g_{l \nu \varphi d}$ in equation (6) are defined as the double integral over the angles $(\theta, \phi)$ of the product of the angular part of derivative of the Green’s function $g$ and the conjugate of the spherical harmonics $Y_{lm}^*$. The function $g(\theta, \phi)$ is evaluated by the method above at discrete grid points on the unit sphere into a grid where the angles $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$ are discretized. For each pair of angles, the integral in equation (5) is computed numerically as described in the previous paragraph. The double integral in equation (6)
over $\phi$ is computed using the trapezoidal rule, and the integral over $\theta$ is computed using Gauss quadrature to obtain the expansion coefficients. The accuracy of the calculations for the expansion coefficients $g_{lm}$ depends on the number of grid points chosen for discretizing the function on the unit sphere. Figure 3(b) shows how the error between computing $g$ in equation (4) and its expansion in spherical harmonics in equation (5) varies as a function of the number of angles $(\theta, \phi)$ chosen. For about $150 \times 150$ grid points, 13 decimal places can be achieved.

In application, the spherical harmonics series used to describe the stress (equation (12)) or the force (equation (13)) must be truncated. The truncation number is denoted by $q_{\text{max}}$. The larger the expansion order $q_{\text{max}}$ considered in the series, the more accurate and more expensive the calculations of stress and force become. For instance, if the material is isotropic, i.e. has a coefficient of anisotropy

$$A = \frac{2C_{44}}{C_{11} - C_{22}}$$

of 1, then truncating the series at $q_{\text{max}} = 1$ gives the exact solution. For all the anisotropic ratios, the solution becomes approximate but fully precise.

The error in the force calculation is evaluated by computing how much accuracy is gained by adding a new term in the spherical harmonics series. This error is defined as the average between the relative error on the four norms of the force on the four nodes of two interacting orthogonal segments, each of length $L = 100$ and separated by a distance of $d = 10$ in arbitrary units. The error is computed such that

$$\delta F_{\text{error}}(q) = \frac{1}{4} \sum_{i=1}^{4} \frac{|F^q_i - F^{q+1}_i|}{|F^q_i|}.$$

The main cost of the interaction force or stress calculations resides in the calculations of the integrals $J, H$ (see equations (14)–(15)) as everything else can either be precomputed independently of the two segment lengths and directions or computed efficiently using the contracted matrices $A$ and $B'$ as defined in section 3. Figure 4(a) shows the time spent in computing forces as $q_{\text{max}}$ increases for a fixed anisotropy ratio of $A = 0.1$. That cost is computed as the time spent to compute force for a particular $q_{\text{max}}$ versus the time spent...
to compute the same forces using isotropic elasticity, i.e. $q_{\text{max}} = 1$. The polynomial fit of figure 4(a) shows that this cost is quadratic in $q_{\text{max}}$.

The expansion order $q_{\text{max}}$ needed to compute forces accurately is related to the anisotropy of the elastic media. As the anisotropy increases, more coefficients in the spherical harmonics series are needed to reach a given accuracy. Figure 4(b) shows how the error in force calculations varies as a function of increasing anisotropy $A$ and cost. This cost in turn is related to $q_{\text{max}}$. For $A = 1$, the isotropic case, the error in the force calculations is $10^{-16}$ for $q_{\text{max}} = 1$. For $A = 7.4$, corresponding to $\alpha$-Fe at 900°C, an error of $3 \times 10^{-6}$ is reached for $q_{\text{max}} = 20$ and is 56 times more expensive than isotropic elasticity.

Figure 5(a) shows how the error in force calculations decreases with the expansion order $q_{\text{max}}$ in the spherical harmonics series for a few values of anisotropy ratio $A$. This decrease is exponential. The convergence rate can be fitted as a function of $\log A$. Figure 5(b) shows a numerical fit of the form $-\exp[-(\alpha \log A + \beta)^{\gamma}]$. Parameters $\alpha$, $\beta$ and $\gamma$ differ slightly between the right and left fits of the data and are given by $\alpha = 0.82$ and $-0.87$, $\beta = -0.04$ and 0.01, and $\gamma = 2.2$ and 1.6 for the left and right fits, respectively. In summary, the log of the error in force calculations varies as $-\exp[-(\alpha \log A + \beta)^{\gamma}]q_{\text{max}}$ where $A$ is the anisotropy ratio and $q_{\text{max}}$ is the expansion order.

The convergence of the spherical harmonics series also depends on the geometry of the two interacting segments. We consider the same two non-parallel segments as before but now we vary the distance $d$ between the two segments. The error made by computing the interaction forces as a function of distance $d/L$ is shown in figure 6 for three different anisotropic coefficients of 1.0, 3.7 and 7.4 going from no, intermediate to large anisotropy. The error in force calculations does not strongly depend on the distance between the two segments.

The cost and accuracy for the calculation of a stress at a point, equation (12), as $q_{\text{max}}$ and $A$ increase are also analyzed. The same qualitative behavior exhibited by the interaction force between two segments is observed for the computation of the stress at a point on one segment coming from the other segment.

5. Discussions and conclusion

Dislocation dynamics (DD) simulations involve heavy calculations. To account for hardening and dislocation patterning and avoid small volume artifacts, DD simulations require several
Figure 6. Convergence of the error in force calculations as a function of the distance $d$ separating the two interacting segments of fixed length $L = 100$ for three anisotropic ratios. The error in force calculations remains stationary with increasing relative distance between the two dislocation segments.

millions of dislocation segments and millions of steps to reach the strain levels at which the hardening transitions are observed in isotropic elasticity, i.e. 1–2% of strain [16]. At each step of segment–segment interactions, dislocations are computed analytically when the segments are close to each other and using the fast multipole method when they are far away [11]. The calculations of the interaction force between two segments or the stress between a point and a segment are the most repeated and expensive parts of a DD simulation.

The interaction force between two dislocation segments in anisotropic elasticity has been computed using either the Brown or the Willis–Steeds formalisms in previous works [5, 10]. Using these methods, the stress is integrated numerically at Gauss quadrature points on the dislocation segments and then summed up to get the force at the end nodes of the two segments. This method performs better when the two segments are far apart. As the segments get close to each other, more integration points are necessary to retain the accuracy of the force. Numerically integrating over segments has been found to be expensive in DD simulations. Rhee et al [5] reported that this method is 500 times more expensive than the equivalent calculation in isotropic elasticity. Yin et al [10] were able to reduce the cost and reported a cost of 220 for using anisotropic elasticity versus isotropic elasticity for tungsten. The variability of the costs reported is not surprising given that Arsenlis et al [11] showed that the cost of numerical integration could vary by orders of magnitude depending on the separation of the line segments in isotropic elasticity.

Using an expansion in spherical harmonics series for the derivative Green’s function allows for analytical integration over a segment for the stress at a point and over two segments for the force. The accuracy of this decomposition does not depend on how many integration points are chosen to evaluate integrals but rather on the order of truncation in the spherical harmonics series, which can be chosen to specify a predetermined accuracy for a given level of elastic anisotropy. Analytical integration overcomes deterioration of accuracy of the calculations as the segments get closer.

In isotropic elasticity, an analytical expression to compute the forces between interacting pairs of segments is given in Arsenlis et al [11]. A calculation of the number of operations between analytically computing forces in isotropic, as defined in [11], and anisotropic elasticity using spherical harmonics series shows that there are about 850 multiplications, 600 additions and subtractions, and about 60 other operations such as logs, square roots, divisions and arc tangents for isotropic elasticity versus about 2450 multiplications, 1300 additions and
Figure 7. Force calculation error between two non-parallel segments of length $L = 100$ and separated by a distance $d = 10$ as the expansion order $q_{\text{max}}$ in the spherical harmonics series is set to 21. The error in force calculation does not exceed $10^{-4}$.

subtractions, and 40 other operations in anisotropic elasticity for $q_{\text{max}} = 1$. Since cost comparisons between two different codes can vary significantly with different compilers, if we were to estimate a cost similar to that previously reported in the literature, for our new method, we could amplify the relative cost reported in figure 4(a) by a factor 1.5–3.

As explained in Arsenlis et al [11], the cost of computing interaction forces is balanced out between near- and far-field interactions in a DD simulation. A typical DD simulation domain is decomposed into cells. For two cells in the simulation domain, the interaction force between dislocations within those cells is computed either by using direct calculation of the forces or using the fast multipole method. The distance between two cells determines which method is used. Local interactions scale as $O(n^2)$ and far away interactions scale as $O(N)$ where $N$ is the total number of segments in the simulation and $n$ is the number of segments per cell. An optimal choice of the number of cells and the ratio of $n/N$ can be computed to decrease the cost of local anisotropic calculations. Assuming that the cost of the fast multipole method is comparable between isotropic and anisotropic elasticity, then the total cost of the calculation would increase by the square root of the cost factors discussed because the fraction of near field to far field would be rebalanced to optimize the total force calculation.

The convergence of the log of the error in the force calculations decreases linearly with the expansion order $q_{\text{max}}$ in the spherical harmonics series. As $q_{\text{max}}$ increases, the terms in the coefficients $Q_m^n(k)$ grow quickly. When using double precision to store numbers, a lack of precision in the calculations starts to appear for $q_{\text{max}} > 21–25$. This instability is due to the explicit description of the associated Legendre polynomials into a product of $S$ and $H$. Nevertheless, in our simulations, $q_{\text{max}} = 21$ corresponds to an accuracy in force calculations that does not exceed $10^{-4}$. Figure 7 shows the error in force calculation when $q_{\text{max}}$ is fixed to 21. In practice, $q_{\text{max}}$ may not go beyond 10 or so. One way to improve the limitation in the expansion order in the spherical harmonics would be to increase the rate of convergence of the error. For instance, polynomials other than Legendre may converge faster with increasing expansion order.

Acknowledgments

The Lawrence Livermore National Laboratory is operated by the Lawrence Livermore National Security, LLC, for the US Department of Energy, National Nuclear Security Administration, under Contract DE-AC52-07NA27344.
Appendix

The following sections describe how to determine the single integral for computing the stress at a point coming from a dislocation segment in the case where the point is collinear to the segment or not. The double integral involved in the computation of the force is determined in the case of two collinear, parallel and non-parallel dislocation segments.

Appendix A. Analytical evaluation of the stress at a point due to a finite segment

The stress at a point \( x \) coming from a segment \([x_1, x_2]\) with line direction \( t' \) that does not contain \( x \), equation (12), is

\[
\sigma_{js} = \epsilon n_{gs} C_{jsg} C_{pdws} b^2 \sum_{q=0}^{\infty} \sum_{m=-q}^{q} \Re \left( S_{\text{pm}}^{\text{sn}} f_{m,(2q+1-m),2q+3} \right) \tag{A.1}
\]

where the single line integral \( \tilde{J}_{ijk} \) is defined as

\[
\tilde{J}_{ijk} = J_{ijk}(x - x_2) - J_{ijk}(x - x_1)
\]

where

\[
J_{ijk}(R) = \int K_{ijk}(R) \, dr \quad \text{and} \quad K_{ijk}(R) = \frac{(R \cdot e_{12})(R \cdot e_3)^j}{R^2},
\]

\( R \) is the distance between \( x \) and the segment \([x_1, x_2]\). The definition of \( r \) depends on the geometry of the finite segment.

A.1. Evaluation of analytical integrals for a non-collinear segment

The stress at a point \( x \) coming from a non-collinear segment is given in equation (A.1) for \( R = rt' + du \) with \( r = R \cdot t' \) in \([r_1, r_2]\) where

\[
r_1 = (x - x_1) \cdot t', \quad r_2 = (x - x_2) \cdot t', \quad u = \frac{R - R \cdot t'}{|R - R \cdot t'|} \quad \text{and} \quad d = R \cdot u.
\]

\( R \) is the norm of \( R \), and \( i + j = k - 2 \) where \( k > 1 \) is odd.

The single integral \( J_{ijk}(R) \) can be calculated via recurrence. The initial terms of \( J_{ijk}(R) \) to start the recurrence are \( J_{(i-1)jk} = J_{(i-1)jk} = 0 \) and

\[
J_{001} = \ln(R + R \cdot t')
\]

\[
J_{011} = \beta R + \gamma J_{001}
\]

\[
J_{011} = \epsilon R + \theta J_{001}.
\]

The higher order terms are

\[
J_{ij(k+2)} = \frac{1}{k d^2} \left[ (k - i - j - 1) J_{ij} + (R \cdot t') K_{ijk} + i \beta J_{ij-1} + j \theta J_{ij-1} \right]
\]

\[
J_{i(j+1)k+2} = \frac{\epsilon}{k} \left[ i \beta J_{i(j-1)k} + j \epsilon J_{ij-1} - K_{ijk} + \theta J_{ij} \right]
\]

\[
J_{i(j+1)k+2} = \frac{\beta}{k} \left[ j \epsilon J_{i(j-1)k} + i \beta J_{ij-1} - K_{ijk} + \gamma J_{ij} \right]
\]

where \( \beta = t' \cdot e_{12}, \epsilon = t' \cdot e_3, \gamma = d u \cdot e_{12} \) and \( \theta = d u \cdot e_3 \).
A.2. Evaluation of analytical integrals for a collinear segment

In the collinear case, where \( x \) does not intersect the dislocation segment \([x_1, x_2]\), the single integral \( J_{ijk}(R) \) can be expressed explicitly and is given for \( i + j = k - 2 \), with \( k \) odd and greater than 1, and \( r = R \cdot t' \) by

\[
J_{ijk} = (t' \cdot e_{12})^i (t' \cdot e_3)^j \int \frac{r \, dr}{|r|^3} = -\frac{\beta^i e^j}{R}.
\]

Appendix B. Analytical evaluation of the interaction forces between two finite segments

The interaction force between two segments \([x_1, x_4]\) and \([x_1, x_2]\) evaluated at the end node \( x_4 \), with line directions \( t \) and \( t' \) and lengths \( L \) and \( L' \), respectively, equation (13), can be expressed as

\[
F_i^3 = \frac{1}{L} \epsilon_{ij0} \epsilon_{mnr} C_{jxvg} C_{pdvn} b_j b'_n t_o t'_r \\
\sum_{q=0}^{\infty} \sum_{m=0}^{2q+1} \Re \left( S_{vpd}^{qm} [H_{m,(2q+1-m),2q+3} - s_3 H_{m,(2q+1-m),2q+3}] \right), \quad (B.1)
\]

The interaction forces evaluated at the other end nodes \( x_1, x_2 \) and \( x_1 \) of the two segments are

\[
F_i^3 = \frac{1}{L} \epsilon_{ij0} \epsilon_{mnr} C_{jxvg} C_{pdvn} b_j b'_n t_o t'_r \\
\sum_{q=0}^{\infty} \sum_{m=0}^{2q+1} \Re \left( S_{vpd}^{qm} [H_{m,(2q+1-m),2q+3} - s_3 H_{m,(2q+1-m),2q+3}] \right)
\]

\[
F_i^2 = \frac{1}{L} \epsilon_{ij0} \epsilon_{mnr} C_{jxvg} C_{pdvn} b_j b'_n t_o t'_r \\
\sum_{q=0}^{\infty} \sum_{m=0}^{2q+1} \Re \left( S_{vpd}^{qm} [H_{m,(2q+1-m),2q+3} - r_2 H_{m,(2q+1-m),2q+3}] \right)
\]

\[
F_i^1 = \frac{1}{L} \epsilon_{ij0} \epsilon_{mnr} C_{jxvg} C_{pdvn} b_j b'_n t_o t'_r \\
\sum_{q=0}^{\infty} \sum_{m=0}^{2q+1} \Re \left( S_{vpd}^{qm} [r_1 H_{m,(2q+1-m),2q+3} - H_{m,(2q+1-m),2q+3}] \right)
\]

respectively.

These forces are expressed using the three double line integrals \( H_{ijk}(R), H^r_{ijk}(R) \) and \( H^s_{ijk}(R) \) using

\[
[H_{ijk}(x_4 - x_2)] = H_{ijk}(x_4 - x_2) - H_{ijk}(x_4 - x_2) - H_{ijk}(x_4 - x_1) + H_{ijk}(x_4 - x_1)
\]

\[
[H^r_{ijk}(x_4 - x_2)] = H^r_{ijk}(x_4 - x_2) - H^r_{ijk}(x_4 - x_2) - H^r_{ijk}(x_4 - x_1) + H^r_{ijk}(x_4 - x_1)
\]

\[
[H^s_{ijk}(x_4 - x_2)] = H^s_{ijk}(x_4 - x_2) - H^s_{ijk}(x_4 - x_2) - H^s_{ijk}(x_4 - x_1) + H^s_{ijk}(x_4 - x_1)
\]

where

\[
H^s_{ijk}(R) = \int \int K_{ijk}(R) s \, ds \, dr, \quad H^r_{ijk}(R) = \int \int K_{ijk}(R) r \, ds \, dr
\]

\[
H_{ijk}(R) = \int \int K_{ijk}(R) ds \, dr.
\]

The definitions of \( r \) and \( s \), \( r_1 \), \( r_2 \), \( s_3 \) and \( s_4 \) depend on the geometry of the two interacting segments.
B.1. Evaluation of analytical integrals for two non-parallel segments

The interaction force between two non-parallel, non-intersecting and non-collinear dislocation segments is given by equation (B.1) for $\mathbf{R} = s\mathbf{t} + r\mathbf{t}' + \mathbf{d}\mathbf{u}$ with $s$ in $[s_3, s_4]$ and $r$ in $[r_1, r_2]$ with

$$\mathbf{u} = \frac{\mathbf{t} \times \mathbf{t}'}{|\mathbf{t} \times \mathbf{t}'|}, \quad d = \mathbf{R} \cdot \mathbf{u}, \quad s = \frac{\mathbf{R} \cdot (\mathbf{t} - \mathbf{t}')}{1 - c^2}, \quad r = \frac{\mathbf{R} \cdot (\mathbf{t}' - \mathbf{c})}{1 - c^2} \quad \text{and} \quad c = \mathbf{t} \cdot \mathbf{t}'.$$

The bounds of $r$ and $s$ are defined by

$$s_3 = \frac{(x_3 - x_4) \cdot (t - ct')}{1 - c^2}, \quad s_4 = \frac{(x_4 - x_3) \cdot (t - ct')}{1 - c^2},$$

$$r_1 = \frac{(x_3 - x_4) \cdot (t' - ct)}{1 - c^2}, \quad r_2 = \frac{(x_4 - x_3) \cdot (t' - ct)}{1 - c^2}.$$

The double integrals $H_{ijk}^r(\mathbf{R})$, $H_{ijk}^l(\mathbf{R})$ and $H_{ijk}(\mathbf{R})$ can be expressed using recurrence relations. The initial terms to start the recurrence are $H_{i(-1)jk} = H_{(i-1)jk} = H_{i(-1)jk} = H_{(i-1)jk}^r = H_{(i-1)jk}^l = 0$ and

$$H_{003} = \frac{2}{\sqrt{d^2(1 - c^2)}} \tan^{-1} \left( \frac{(1 + c)(R + r + s)}{\sqrt{d^2(1 - c^2)}} \right),$$

$$H_{003}^r = \frac{cJ_{001}^r - J_{001}^r}{1 - c^2},$$

$$H_{003}^l = \frac{cJ_{001}^l - J_{001}^l}{1 - c^2},$$

and

$$H_{013}^r = \alpha I_{003} + \beta I_{113} + \gamma H_{003},$$

$$H_{013}^l = \delta I_{003} + \epsilon I_{113} + \theta H_{003},$$

$$H_{013} = \alpha I_{113} + \beta I_{023} + \gamma H_{003},$$

$$H_{013}^l = \delta I_{113} + \epsilon I_{023} + \theta H_{003},$$

where we have defined

$$I_{113} = -\frac{R - cd^2H_{003}}{1 - c^2},$$

$$I_{023} = rJ_{001}^r + \frac{cR - d^2H_{003}}{1 - c^2},$$

$$I_{023} = sJ_{001}^l + \frac{cR - d^2H_{003}}{1 - c^2}.$$

The high order terms are

$$H_{ij(k+2)}^r = \frac{1}{k(1 - c^2)} \left[ i(\alpha - c\beta)H_{i(j-1)jk} + j(\delta - c\epsilon)H_{i(j-1)jk} - J_{ijk}^r + cJ_{ijk}^r \right],$$

$$H_{ij(k+2)}^l = \frac{1}{k(1 - c^2)} \left[ i(\beta - c\alpha)H_{i(j-1)jk} + j(\epsilon - c\delta)H_{i(j-1)jk} - J_{ijk}^l + cJ_{ijk}^l \right],$$

$$H_{ij(k+2)} = \frac{1}{kd^2} \left[ sJ_{ijk}^r + rJ_{ijk}^l + iyH_{i(j-1)jk} + j\theta H_{i(j-1)jk} - (2 + i + j - k)H_{ijk} \right],$$

$$H_{i(k+1)jk} = \alpha H_{ijk}^r + \beta H_{ijk}^l + \gamma H_{ijk},$$

$$H_{i(k+1)jk} = \delta H_{ijk}^r + \epsilon H_{ijk}^l + \theta H_{ijk}.$$
and where we have noted \( \alpha = t \cdot e_{12}, \beta = t' \cdot e_{12}, \gamma = du \cdot e_{12}, \delta = t \cdot e_5, \epsilon = t' \cdot e_3, \theta = du \cdot e_3. \)

The single integrals \( J_{i j k}^s (R) \) and \( J_{i j k}^r (R) \) used in the recurrence relations for the double integrals \( H_{i j k} (R), H_{i j k}^s (R) \) and \( H_{i j k}^r (R) \) can also be calculated by recurrence. They are defined as

\[
J_{i j k}^s (R) = \int K_{i j k} (R) \, ds
\]

\[
J_{i j k}^r (R) = \int K_{i j k} (R) \, dr.
\]

The initial terms of \( J_{i j k}^r (R) \) to start the recurrence are \( J_{(−1)j k}^r = J_{(−1)j k}^r = 0 \) and

\[
J_{i01}^r = \ln (R + R \cdot t')
\]

\[
J_{r01}^r = \beta R + ((\alpha - c \beta)s + \gamma) J_{001}^r
\]

\[
J_{0r1}^r = \epsilon R + ((\delta - c \epsilon)s + \theta) J_{001}^r.
\]

The higher order terms are

\[
J_{i(j+1)k+2}^r = \frac{\epsilon}{k} \left[ \beta J_{i(j-1)k}^r + j \epsilon J_{i(j-1)k}^r - K_{i j k} \right] + ((\delta - c \epsilon)r + \theta) J_{i(j+1)k+2}^r.
\]

\[
J_{(j+1)k+2}^r = \frac{\beta}{k} \left[ \epsilon J_{i(j-1)k}^r + i \beta J_{i(j-1)k}^r - K_{i j k} \right] + ((\alpha - c \beta)s + \gamma) J_{i(j+1)k+2}^r.
\]

The line integral \( J^s \) is defined by similar recurrence relations. They are deduced from the recurrence relations of \( J^r \) by replacing \( r \) by \( s, \delta \) by \( \alpha, \epsilon \) by \( \beta, \theta \) by \( \gamma \) and \( t' \) by \( t \).

When the dislocation segments are parallel, \( c = 1 \). The recurrence relations for \( J_{i j k}^s, J_{i j k}^r \) can be simplified and the recurrence relations for \( H_{i j k}, H_{i j k}^s \) and \( H_{i j k}^r \) are not well defined anymore. Recurrences specific to parallel segments are given in the next section.

**B.2. Evaluation of analytical integrals for non-parallel segments**

When two dislocation segments are parallel but not collinear and assuming without loss of generality that their line direction is \( t \), the distance \( R \) is defined as \( R = (r + s) t + du \) where

\[
u = \frac{R - R \cdot t'}{|R - R \cdot t'|}, \quad d = R \cdot u, \quad s = x \cdot t \quad \text{and} \quad r = -x' \cdot t
\]

where \( s \) varies in the interval \([s_3 = x_3 \cdot t, s_4 = x_4 \cdot t]\) and \( r \) varies in the interval \([r_1 = -x_1 \cdot t, r_2 = -x_2 \cdot t]\).

The initial terms to start the recurrence are

\[
H_{003} = \frac{R}{d^2}
\]

\[
H_{003}^s = \frac{1}{2} \left[ \frac{(s - r)}{d^2} R - J_{001}^r \right]
\]

\[
H_{003}^r = \frac{1}{2} \left[ \frac{(r - s)}{d^2} R - J_{001}^r \right].
\]
Low-order terms for $H_{ij}^{\nu}$ and $H_{i}^{\nu}$ are

\[
H_{033}^{\nu} = \alpha I_{023} + \gamma H_{003}^{\nu}
\]

\[
H_{013}^{\nu} = \delta I_{023} + \theta H_{003}^{\nu}
\]

\[
H_{013}^{\nu} = \alpha I_{023} + \gamma H_{003}^{\nu}
\]

\[
H_{013}^{\nu} = \delta I_{023} + \theta H_{003}^{\nu}
\]

where

\[I_{023} = r J_{001}^{\nu} - R\]

\[I_{023} = s J_{001}^{\nu} - R\]

The higher order terms are

\[
H_{ij}^{\nu}(k+2) = \frac{1}{kd^2}[(k - i - j - 2)H_{ij}^{\nu} - H_{ij}^{\nu} + i\gamma H_{(i+1)j}^{\nu} + j\theta H_{ij}^{\nu}]
\]

\[
+ \frac{s}{k - 2}[(i\alpha J_{(i+1)j}^{\nu} - j\delta J_{(i+1)j}^{\nu} - k(R \cdot t)K_{ijk}]
\]

\[
H_{ij}^{\nu}(k+2) = \frac{1}{kd^2}[(k - i - j - 2)H_{ij}^{\nu} - H_{ij}^{\nu} + i\gamma H_{(i+1)j}^{\nu} + j\theta H_{ij}^{\nu}]
\]

\[
+ \frac{r}{k - 2}[(i\alpha J_{(i+1)j}^{\nu} - j\delta J_{(i+1)j}^{\nu} - k(R \cdot t)K_{ijk}]
\]

\[
H_{ij}^{\nu}(k+2) = \delta \left[H_{ij}^{\nu} + j\delta H_{(i+1)j}^{\nu} + i\alpha H_{(i+1)j}^{\nu} - s J_{(i+1)j}^{\nu} + \theta H_{ij}^{\nu}(k+2)
\]

\[
H_{ij}^{\nu}(k+2) = \alpha \left[H_{ij}^{\nu} + j\delta H_{(i+1)j}^{\nu} + i\alpha H_{(i+1)j}^{\nu} - s J_{(i+1)j}^{\nu} + \theta H_{ij}^{\nu}(k+2)
\]

\[
H_{ij}^{\nu}(k+2) = \delta \left[H_{ij}^{\nu} + j\delta H_{(i+1)j}^{\nu} + i\alpha H_{(i+1)j}^{\nu} - s J_{(i+1)j}^{\nu} + \theta H_{ij}^{\nu}(k+2)
\]

\[
H_{ij}^{\nu}(k+2) = \alpha \left[H_{ij}^{\nu} + j\delta H_{(i+1)j}^{\nu} + i\alpha H_{(i+1)j}^{\nu} - s J_{(i+1)j}^{\nu} + \theta H_{ij}^{\nu}(k+2)
\]

In the parallel case, the initial terms of $J_{ij}^{\nu}$ to start the recurrence are $J_{ij}^{\nu}(1) = 0$ and

\[
J_{ij}^{\nu} = \ln(R + R \cdot t)
\]

\[
J_{ij}^{\nu} = \beta R + \gamma J_{ij}^{\nu}
\]

\[
J_{ij}^{\nu} = \epsilon R + \theta J_{ij}^{\nu}
\]

The higher order terms are

\[
J_{ij}^{\nu}(k+2) = \frac{1}{kd^2}[(k - i - j - 2)J_{ij}^{\nu} + (R \cdot t)K_{ij} + i\gamma J_{(i+1)j}^{\nu} + j\theta J_{ij}^{\nu}]
\]

\[
J_{ij}^{\nu}(k+2) = \frac{\epsilon}{\beta} \left[i\beta J_{ij}^{\nu} + j\epsilon J_{(i+1)j}^{\nu} - K_{ij}^{\nu} + \theta J_{ij}^{\nu}(k+2)
\]

\[
J_{ij}^{\nu}(k+2) = \frac{\beta}{\epsilon} \left[j\epsilon J_{ij}^{\nu} + i\beta J_{(i+1)j}^{\nu} - K_{ij}^{\nu} + \gamma J_{ij}^{\nu}(k+2)
\]

\[17\]
B.3. Evaluation of analytical integrals for two collinear segments

When two dislocation segments are collinear and do not intersect, the integrals $H_{ijk}$, $H'_{ijk}$ and $H''_{ijk}$ can be evaluated explicitly. These are given for $i + j = k - 2$, with $k$ odd and greater than 1, $R = (r + s) t$ where $s$ varies in the interval $s_3 = x_3 \cdot t$, $s_4 = x_4 \cdot t$ and $r$ varies in the interval $r_1 = -x_1 \cdot t$, $r_2 = -x_2 \cdot t$ by

$$H_{ijk} = (t \cdot e_{12})^j (t \cdot e_3)^i \int \int \frac{(r + s) \, ds \, dr}{|r + s|^3} = -\alpha^j \delta(i s + r + s) \ln \frac{R}{R'},$$

$$H'_{ijk} = (t \cdot e_{12})^j (t \cdot e_3)^i \int \int \frac{s(r + s) \, ds \, dr}{|r + s|^3} = -\alpha^j \delta(i s + r + s) \ln \frac{R}{R'},$$

$$H''_{ijk} = (t \cdot e_{12})^j (t \cdot e_3)^i \int \int \frac{r(r + s) \, ds \, dr}{|r + s|^3} = -\alpha^j \delta(i s + r + s) \ln \frac{R}{R'}.$$

References


