MATLAB MODELING OF COMPOSITES REINFORCED BY MICRO-NANO PARTICLES

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Abstract

Modeling of composite materials is nowadays a topic which is popular amongst many researchers especially when it comes to materials which are stiffened by micro-nano particles. Accurate simulation of such materials is a cumbersome task since there can be millions of particles in small volume and by such dimensions relatively large to the size of particles the local effects near the particles are hard to catch using existing methods and techniques. Therefore it is imperative to develop multi-scale method which will be able to accurately model local effects and particle interactions on micro-scale and effectively allow to model global behavior of material on macro-scale. The paper presents a continuum model for deformation of material reinforced with cylindrical fibers or tubes with considerably higher stiffness than the matrix. In present models, the inclusions are modeled by dipoles/dislocations, which introduce an asymptotic solution of interaction of the reinforcing fibers and the matrix. Both reinforcing effect of a single inclusion and the interaction of reinforcing particles are important effects in the computational model and in order to increase the efficiency of the model, they are simulated in different level models. The present paper introduces an efficient continuous model for the interaction of a fiber with matrix. The fiber is modeled by distributed forces (Kelvin solution) and by point dislocation along the fiber axis.

1 Introduction

Composite materials reinforced by stiff particles have considerably augmented properties like strength, wear resistance, thermal properties and so on. Computational modeling can be helpful in developing and designing of new materials with never before seen properties. We will present a continuum model for deformation of material reinforced by tubes/fibers where the length compared to diameter is several dozen times larger. Some authors have presented procedures to model composite behavior using BEM/FEM method by which the inclusions were assumed rigid. In our model the inclusions are modeled by fundamental solutions in source points along fiber axis. We will evaluate results using point force acting in one point of nonbounded continuum and dislocation. Both of the functions give asymptotic solution which represents the interaction between the particle and the matrix. We assume that the cohesion between the particle and matrix is large enough so there will not come to their separation. The intensity of a dipole composed from two forces acting on the same line in opposite direction is given by the stress field and deformation in the matrix and will be dependent on material stiffness of inclusion and matrix. To correctly model the local effects near the inclusion we use two scales. On the micro-scale the model enables to obtain the unknown intensities of the dipoles in dependence on local structure and distribution of particles. On the macro-scale the solution simulates global behavior of the structure, i.e. the far field effects. This enables to solve efficiently structures with large number of particles.

In the present paper an efficient continuous model for the interaction of a fiber with matrix is introduced. The fiber is modeled by distributed forces (Kelvin solution), or by point dislocation along the fiber axis. The fiber is supposed to be rigid and its cross sectional dimensions are much smaller than its length. Under such assumptions the number of unknowns can be considerably reduced. The far field action can be then introduced by a single dipole.

2 Modeling of rigid inclusions in elastic field

The inclusions are assumed to be much stiffer than the matrix and the material of the matrix is linear elastic in the present model. As there are large gradients in displacement, strain and stress fields, methods like FEM are inefficient. More suitable are BEM and mesh-less methods. We will use Boundary Point Method (BPM) [1, 2] which we have recently developed for these purposes. This method uses arbitrary Trefftz functions (functions that satisfy governing equation (1), but not necessary boundary conditions), for approximations of field variables in given material. The governing equation expressed through displacements can be written in the following form

$$(\lambda + \mu)u_{j,ij} + \mu u_{i,jj} = 0 \tag{1}$$

where λ and μ are Lame material constants. The equation describes behavior of material under static load conditions.

The macroscopic model of the structure is defined by the elastic matrix and the inclusion is modeled by source points along the axis of inclusion in which either a point forces or dislocations are acting. We have only taken forces and dislocations acting in axial direction of the inclusion as the effects of radial component are only local, they are much smaller than the axial components and can be neglected.

The model of the inclusion is in fig. 1.

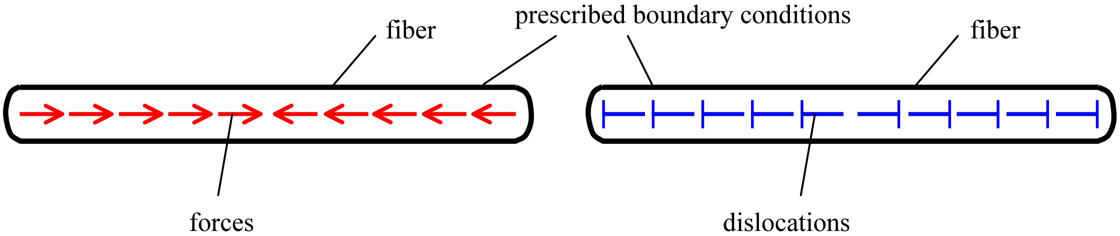

Figure 1: Modeling of a fiber

The displacements, tractions and stresses caused by the unit force acting in a point in space are given by the Kelvin (fundamental) solution as

$$U_{ki} = -\frac{1}{16\pi(1-\nu)Gr^2}\left[\left(3r_{,k}^2 - 1\right)r_{,i} + 2(1-2\nu)r_{,k}\delta_{ik}\right] \tag{2}$$

$$T_{ki} = -\frac{2}{8\pi(1-\nu)r^3}\left[(1-2\nu)\left(2\delta_{ik}n_k + 3r_{,k}^2 n_i - n_i\right) + 6\nu r_{,k}\left(r_{,n} + r_{,i}n_k\right) + 3\left(1-5r_{,k}^2\right)r_{,i}r_{,n}\right] \tag{3}$$

$$S_{kij} = -\frac{2}{8\pi(1-\nu)r^3}\left[(1-2\nu)\left(2\delta_{ik}\delta_{jk} + 3r_{,k}^2\delta_{ij} - \delta_{ij}\right) + 6\nu r_{,k}\left(r_{,j}\delta_{ik} + r_{,i}\delta_{jk}\right) + 3\left(1-5r_{,k}^2\right)r_{,i}r_{,j}\right] \tag{4}$$

where *i, j, k = 1, 2, 3* and *G* and *ν* are shear modulus and Poisson ratio of the material without summation convection over repeated indices, but

$$r = \left[(x_i - y_i)(x_i - y_i)\right]^{1/2} \tag{5}$$

with summation over repeated indices and

$$r_{,i} = \frac{\partial r}{\partial x_i} = \frac{x_i}{r} . \tag{6}$$

All displacement, stress and traction fields are singular, the first two with strong ($1/r^2$) and the third with hyper-singularities ($1/r^3$). In accordance to the definition, it will be the T-function, if the source point where the force act (and so the singularity), is outside the region of the observed body.

Similarly the displacement field caused by the dislocation is given by

$$U_{kij} = \frac{1}{8\pi(1-\nu)r^2}\left[(1-2\nu)\left(\delta_{ji}r_{,k} - \delta_{ki}r_{,j} - \delta_{kj}r_{,i}\right) - 3r_{,k}r_{,i}r_{,j}\right]. \tag{7}$$

Using the T-functions, the displacements in the whole observed domain can be expressed as

$$u_j = U_{ij} f_i \qquad \text{or in the matrix notation } \boldsymbol{u} = \boldsymbol{U}^T \boldsymbol{f} \tag{8}$$

where U_{ij} denotes the i-th T-function and f_i is its intensity, which has to be computed.

The problem is formulated as follows: Find the distribution of forces or dislocations so that the boundary conditions (in displacements in the direction of the fiber axis) on the domain and inter-domain (on the inclusions) boundaries will be satisfied. The unknown intensities f are computed from boundary value problem with prescribed displacements $\overline{u}$ on the inclusion boundary as

$$f = U^{T^{-1}} \overline{u} . \tag{9}$$

Because of large gradients, the inclusion is divided onto smaller elements and numerical integration using Gauss quadratures have to be performed for the matrix **U** which contains contributions of T-functions on displacements (fig. 2). We can write this in the form of integral equation as follows

$$U_{ki} = \sum_i \int K(s,t) N(t) q_i dt = \sum_i \sum_j K(s_i, t_j) N_k(t_j) q_k w_j \tag{10}$$

Furthermore the displacements are interpolated in each element by linear shape function N and on n elements in the centre of inclusion one linear shape function is used (fig. 2).

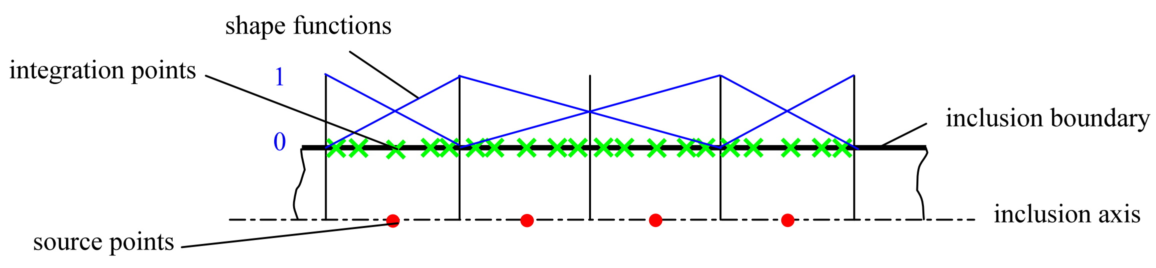

Figure 2: Integration + shape functions

The equation (9) can be solved by the method of least squares (MLS) or singular value decomposition (SVD) [3]. If the number of equations is equal to number of unknowns it really doesn’t matters which one we use for both of methods should return the same results – exact solution. But in case that the matrix is not square the methods act differently. The MLS should smooth the result out by approximating the exact solution in the case of more equations then unknown quantities. SVD solver [3], which was included into the MATLAB [4] gives better results in the case that the matrix has more columns than rows, i.e. more unknowns than equations. All singular values lower than certain tolerance, are ignored.

For a far field action the whole particle model can be reduced to a dipole or a dislocation placed in the centre of the particle with resulting intensity. The tractions, **t**, simulating the action of the rigid particle on the matrix define the *i*-th component of intensity of the dipole as

$$h_i = \int_S y_i t_i dS \tag{11}$$

where the integration is performed over the particle boundary, *S*, and summation convection is not applied in this expression. The intensity of a couple of forces corresponding to the dipole is the product of the force and the distance between the points where the forces act. In our model the resulting intensity of the dipole is defined by intensities of forces applied along the particle axis.

Again equivalent to a dipole is a dislocation. The intensity of a single dislocation is defined simply as integral of distributed intensities along the fiber axis.

3 Discussion and results

MATLAB was used to perform the calculation of dipole and dislocation convenient to model the far fields. The length of the fiber is 500 units and the radius 2 units. The particle is divided onto 160 elements and 5th order Gauss quadrature is used to assemble the matrix of T-functions. There were 160 source points along the inclusion axis. Displacements were prescribed along the particle boundaries and accuracy of solution methods dependent on number of elements approximated by linear shape function was observed. Comparison of the resulting dipole intensity solving with MLS and SVD method is shown in fig. 3. The same comparison, but for the resulting dislocation is in fig. 4.

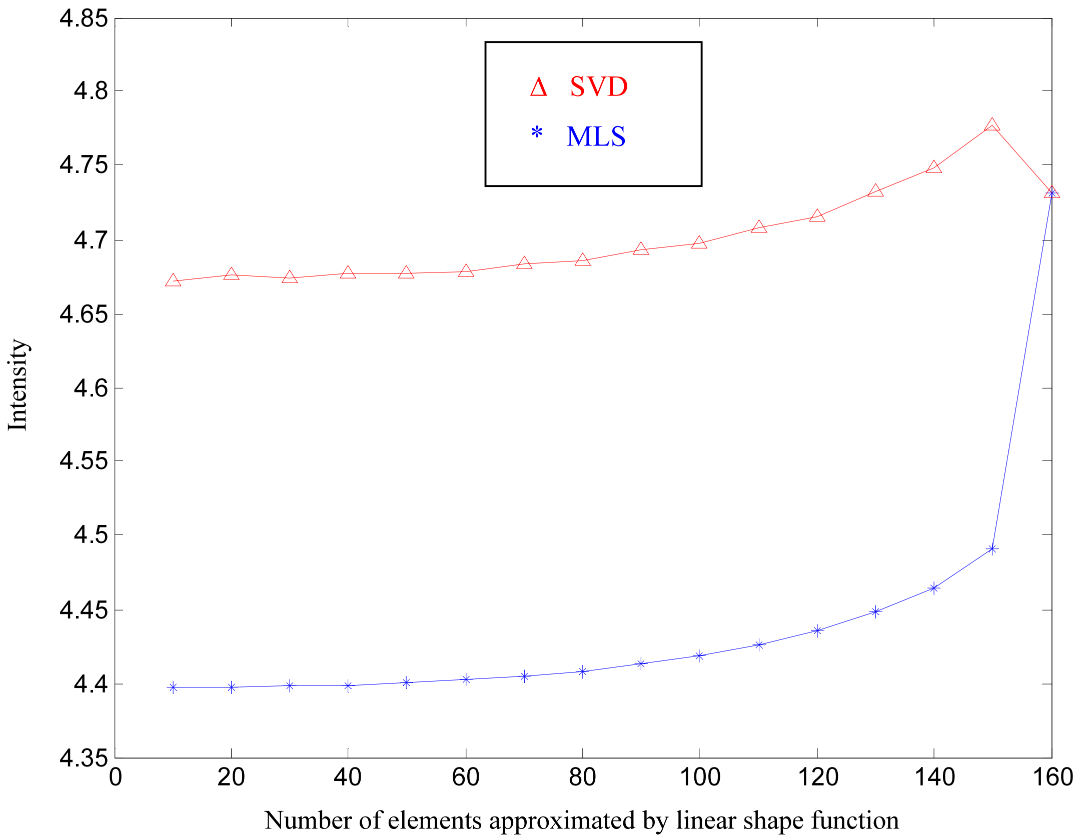

Figure 3: Intensity of resulting dipole

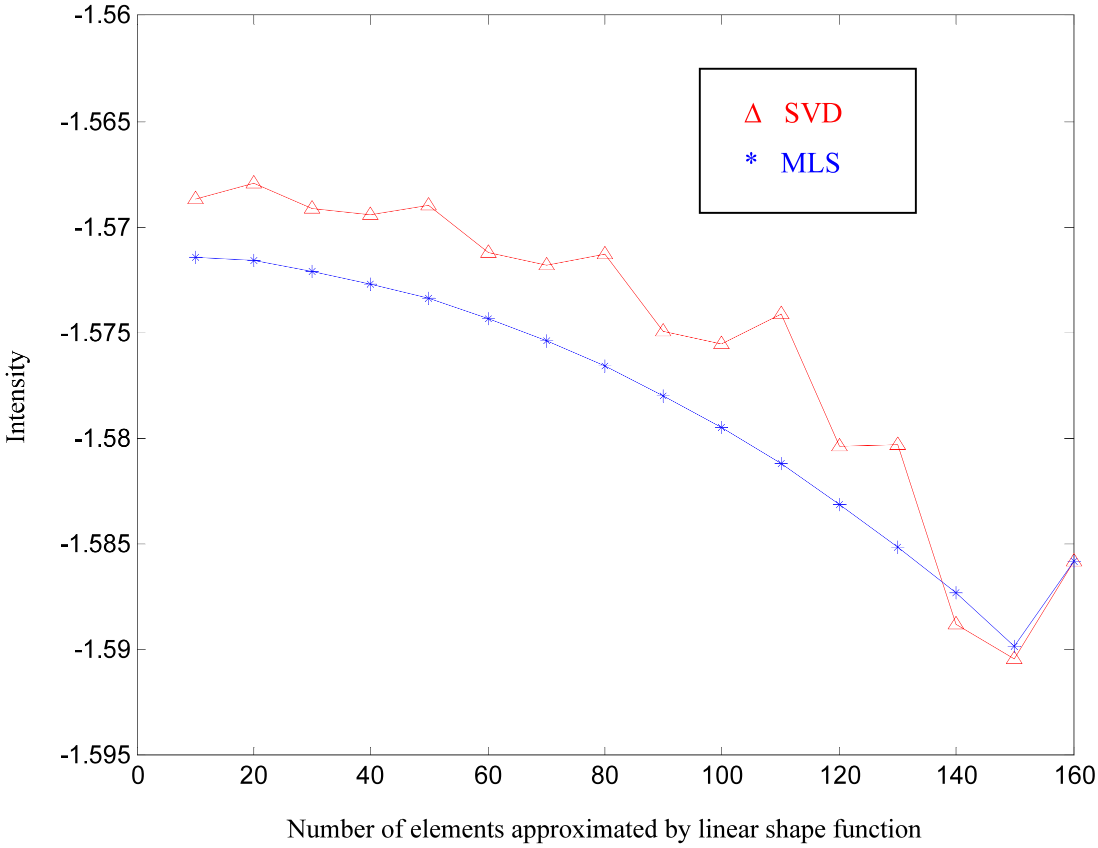

Figure 4: Intensity of resulting dislocation

As can be seen from both fig. 3 and fig. 4 the solving methods behave differently under various circumstances. By the dipole solution more accurate results are given by the SVD method with variation of only 2.2% compared to MLS which results are varying 7.5%. The opposite is true by the dislocation where the MLS gave smooth and more accurate results with variation of only 1.2% compared to SVD where the variation in results is 1.4%. The variation is caused by large gradients especially on the ends of the inclusion where the error in computation is largest.

Next we have examined the distribution of force and dislocation intensities along the particle axis. First we have computed the intensities with collocation method. On fig. 5 we can see that the intensities for both forces and dislocations behave almost linearly along the length of particle except for the ends.

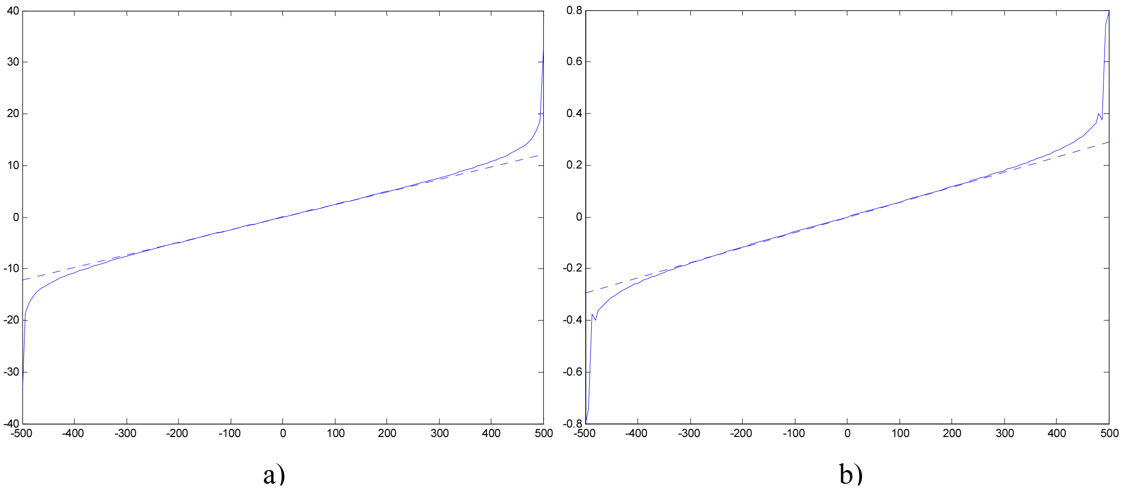

Figure 5: Intensities along the particle axis a) forces b) dislocations

The main idea is that we can simplify the model once more by approximating the intensities by linear shape function. We can do this on the whole length of the inclusion or on a certain interval near the centre of the inclusion and observe how the accuracy of the solution changes. This way we can find an interval with polynomial approximation and still the accuracy will be good and the efficiency will be several times higher. In fig. 6 are intensities along the axis of the inclusion for various intervals on which the solution is approximated by linear shape function where *n* is number of elements sharing the shape function. Note that, on each element the integration was performed using Gauss quadratures.

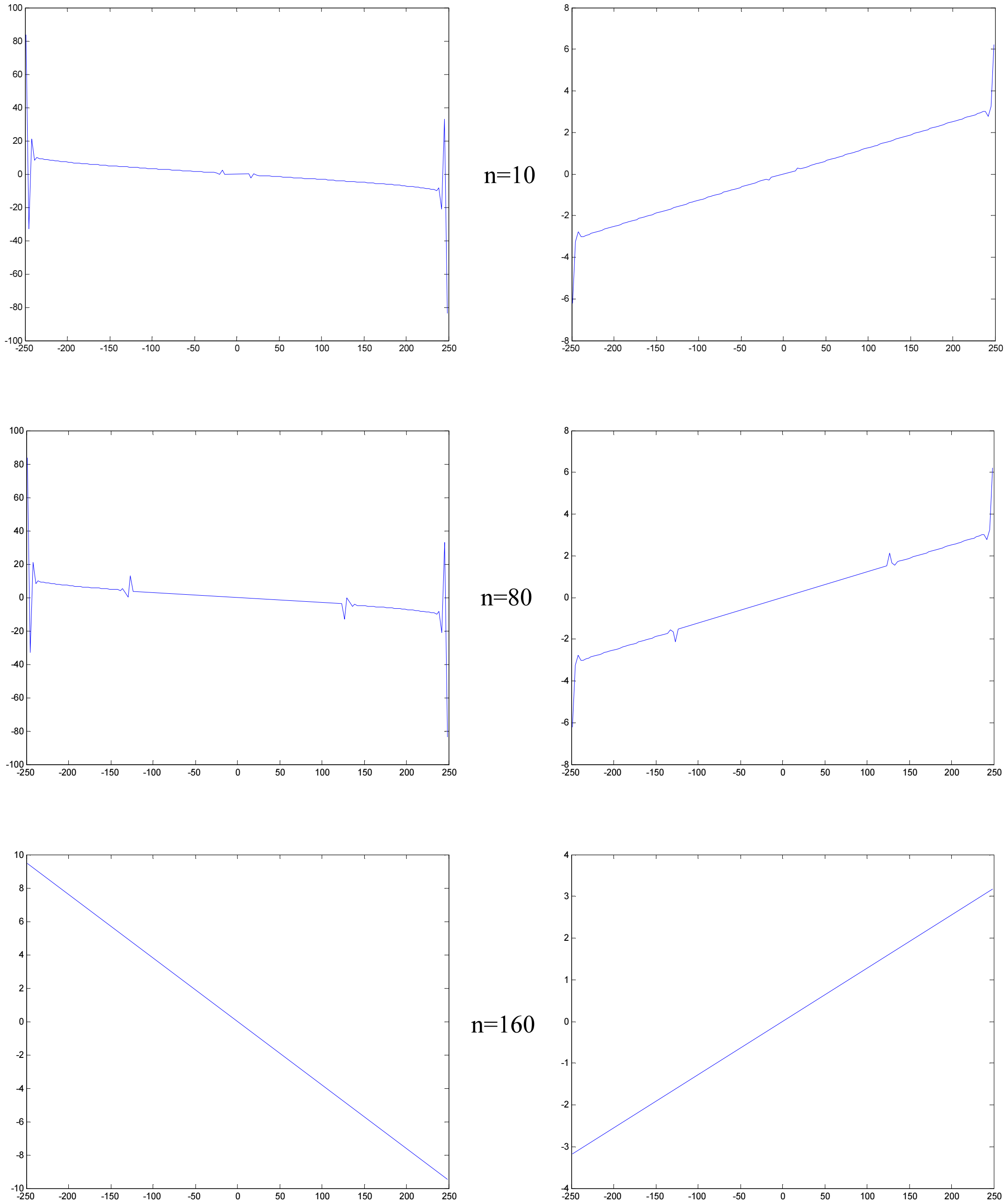

Figure 6: Intensities along the particle axis; left: forces, right: dislocations

From the fig. 6 we can see that on ends and on the outer limits of the interval there are some discontinuities. This is due to larger gradients on the ends and so a numerical error arises. Despite of this the function is quite good approximated by only two points (for n=160), where the shape functions spans the whole length of the particle. Note though that, in this way some large errors occurs on the ends which can be seen in fig. 7. The blue line represents absolute error from prescribed displacements in longitudinal direction, the red line is error from corresponding radial displacements.

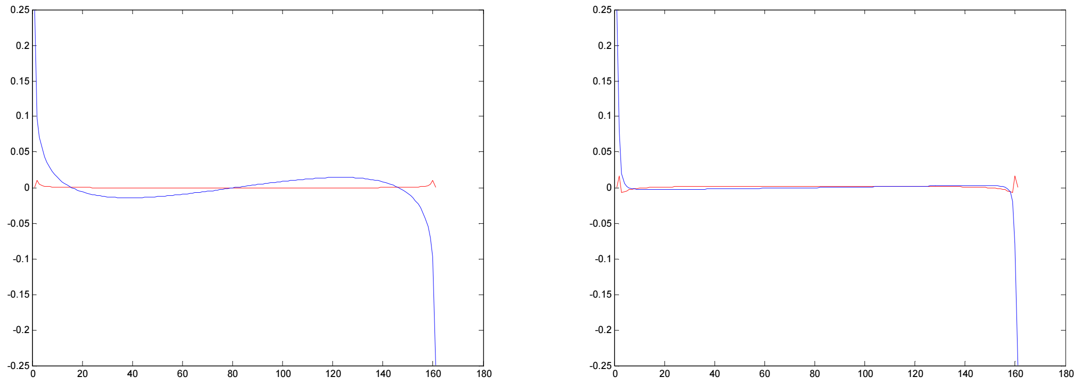

Figure 7: Error in displacements; left: force, right: dislocation

The dislocation model seems to be better suitable as the linear approximation gives very small error in displacements almost on the whole length of the model. The ends need to be modeled in another way as there is more than 80% error from prescribed value. This will be part of the next research.

4 Conclusions

The paper presents numerical model which enables to model rigid inclusions in elastic matrix. It was assumed that the inclusion is much stiffer than the matrix and the cross sectional dimensions of the fiber were much smaller its length. This enables to simplify the model in the way that only the displacement conditions along the fiber axis are satisfied by the model. The other conditions are satisfied approximately, too, as the cross sectional deformations are negligible and the forces, modeling the interaction of the fiber with matrix are in internal equilibrium and dislocations do not introduce any resulting force. For a far field action a procedure is assumed which models each inclusion as a single dipole or a single dislocation with given intensity. This is prerogative if it is to model macro-scale composite material, which contains up to several thousands, or millions of inclusions. This includes high gradients near the inclusions and interaction between all, the matrix and particle, among the particles and particles with the domain boundaries. The method can be extended to more general nonlinear material behavior is simple to model and will not complicate the model much. MATLAB proves to be an excellent tool which helps the developing of complex numerical algorithms.

References

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