Documentation

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Contents

1 README files

1.1 File execution order

InPut files

input and Fracture energy files provide an input numbers for package1 and contains information and it contains primitive information of system geometry and properties.

1.1.1 Interactions: Multipole Method

1. **geometry**: The initial geometry of the system will be defined by running this file. It reads information from input file.

2. **expansionCoefficients**: Employing the information in geometry file, all expansion coefficients (Eta and Mu) are calculated using expansionCoefficients file.

3. **abmnpq**: In this file expansion coefficients of harmonic terms are calculated.

4. **matrix**: After some analytical calculations, the whole problem is reduced to a set of linear system of equations. To solve the system using linear solver, the system has to be write in matrix format.

5. **farfield**: All stress fields in the system have to be expanded in bases of the harmonic terms. Therefore, far field which is uniform here is expanded in terms of harmonic terms in this file.

6. **linearSolve**: In this file, a linear system of equation is solved using Linear solver and results that are expansion coefficients A,B,C, and D are written in the LinearSolve file.

7. **PhiPsi**: Phi and Psi are scalar Muskhelishvili potentials of complex variable method in plane Elasticity. Zero suffix functions denote potentials in the matrix host.

8. **StressFields**: Stress fields in y_q local in z_q local and in z global coordinate system are calculated.

9. **DisplacementFields**: I Have To Check The Correctness Of The Field In The Package.
   Displacement fields in y_q local in z_q local and in z global coordinate system are calculated.

10. **SIF**: I Have To Check The Correctness Of The Field In The Package $K[q]$ and $Kminus[q]$ for each inclusions are calculated in this file. k and $kminus$ show SIF i and ii (mode I and II) for RHS and LHS of the inclusion respectively.

11. **PackageManipulations**: (* :Author:Leonid B.Shifrin*)
    The package provides tools to (dynamically) re-load, clear and/or remove the context of any loaded package (optionally with sub-contexts) during interactive Mathematica session or during execution of a stand-alone program. These operations are performed respecting the general package mechanics in

Mathematica.Additional functionality includes (optional) automatic resolving of shadowing problems that may have occured before or during reloading,and tracking escaping symbols

1.1.2 Crack propagation

1.1.3 File Boundary Element Method

1. **GenerateMesh**: Boundary discretization. Save XY matrix in XY.dat file.

2. **FieldsBE**: Base solution Stress and displacement fields.

3. **CoefMat**: Produce coefficient matrixes Uij and Cij. Save Uij and Cij matrix in Uij.dat and Cij.dat files.

4. **BCSolve**: Form solution matrix Sij depending boundary condition.

5. Define $B.C : s$ vector of $2 * NTOTAL$ elements.

6. Solve $Sij.W = s$ and find W as weight function vector. Save W vector in $W.dat$ file.

7. **FieldsXY**: Substitute W in the new matrix of $Uij(x, y)$ and $Cij(x, y)$ and finding fields using $Uij(x, y).W$ and $Cij(x, y).W$.

1.1.4 Thermal Effects

1.1.5 Dislocation Dynamics

1.1.6 File run

- **CombinMMBE**: In this file a tangential stress field caused by the grain boundary on the premier of the qth inclusion is calculated. This function will be used to find a correct propagation direction in eta0 function in the run2 file.

- **run0**: In this file stress fields of the system are calculated using the multipole method. Then, by using the correct coefficients and removing regular fields (by equating Eta_{nmpq} and Mu_{nmpq}), stress fields can be calculated at any point in the model.

- **run1**: This file produces two matrixes of expansion coefficients; eta and mu.

- **run02**: This file calculates the stress fields caused by the inclusions on the points of the mesh of the grain boundary. This information (SMM) will be used as the supplementary boundary condition for BE method. Then, change expansion coefficient to the original values and combine BE and MM by loading **CombinMMBE** file.

- **run2**: In this file coordinates of the new propagated inclusion are found using the maximum tangential stress criterion. The new coordinate is saved in the output file. It automatically updates the output file.

- **run3**: In this file, the path propagation of an inclined inclusion is calculated. The path propagation is predicted by just adding crack/inclusion and recalculating stress fields between cracks/inclusions.

- **run4**: In this file the path propagation of an inclined inclusion is calculated. The path propagation is predicted by finding an equivalent crack/inclusion and recalculating stress fields between cracks/inclusions.

- **run5**: This file reads output1 and calculates crack propagation path.

- **run1EtaMu0**: Using this file, the full stress field of the system can be calculated.

1.2 README-HowToRunNote.txt

To start running the package,

- you must once use the **initiation.nb** file and run it on your computer. It defines the package folder path to run the program. The file will be created in the home directory of your computer and the main package folder.

- To test and run the package you can use the **DCD_Run.nb** file in the main folder

1.3 README-RunErrorNote

1. ErrorNote1: Part::partw: Part 2 of 0 does not exist.

2. Matrices Eta, Mu are calculated using **run1.m** file. New matrices Eta and Mu have to be recalculated before starting simulation on any new configuration of inclusions. Therefore, the first step for any new configuration is running **run1.m**. Otherwise, the above error will appear.

3. StartNote2: To the start the program, the output file must not be in the folder.

4. ErrorNote2: Some times if the crack is inside the interface layer, the program can not solve it correctly. You must change the crack incremental size to get the correct result.

1.4 README-input-output

- n = It defines the total number of harmonic terms for accuracy of the calculations.
- n1 = Number of initial inclusions in the x direction
- n2 = Number of initial inclusions in the y direction
- ntot= total number of inclusions
- Nu0 = Poisson ratio for the host material
- Mu0 = Shear modulus for the host material
- Uniform Far-field:
  s11
  s12
  s22
- NuQ = Poisson ratio for the inclusions (ntot terms, ntot = number of inclusions)
- MuQ = Shear modulus for the inclusions (ntot terms)
- l1 = Major axis of elliptical inclusions (ntot terms)
- l2 = Minor axis of elliptical inclusions (ntot terms)
- teta = Inclusion's orientation $[-90, 90]$ (ntot terms)
- teta1 = Inclusion's orientation $[0, 360]$(ntot terms)
- zcender = (x+Iy) centre point of each inclusions in global coordinate system.
- zcendernew = centre point of each new created inclusions in global coordinate system.

The input file provides input numbers for package1 (geometry) and contains primitive information of system geometry and properties. The output file has the same information after executing the simulation.

1.5 README-output-files

- **output**: Store information after each simulation step. It should finally contain $ninitial + 1$ inclusions.

- **outputtemp**: Store information about the system configuration after merging two inclusions at each simulation step.

- **output1**: Store all information about the primary inclusions before merging. Crack propagation path and inclination angle changes can be derived from this file.

- **output2**: Delete latest inclusion's information from the **outputtemp** to explicitly present crack propagation with two cracks at each simulation step. Then, **output2** is copied to the output and simulation is run by a higher number of n for obtaining a better accuracy of the system $SIFs$.

- **outputnew**: Information of the new inclusion. I have to check it; seems odd to me!

- **cracktemp**: Contains information of two inclusions that present crack propagation at each step. l1[1], l1[2], l2[1], l2[2], theta[1], theta[2], kminus[1], k[2], kcrack[1], kcrack[2]

- **crack.XLSX** cracktemp file restored in the XLSX and csv file formats.

- **crack.csv**

1.6 README-outputnew

- l1new = Size of new inclusion + delta distance between them
- tetanew = Angle of new inclusion
- zcenternew = centre of new inclusion
- NuQ1temp = 0
- MuQ1temp = 0

1.7 README-FractureEnergy

- G0::usage =”Fracture energy of host material.”;
- GQ::usage =”Fracture energy of inclusions.”;
- kQ::usage =”Surface perfectness of inclusions.”;
- GGB::usage =”Fracture energy of the grain boundaries.”;
- VGB::usage =“Vertices of the grain boundaries.”;
- BE::usage=” If use finite boundary put 1 in the Fracture energy file, otherwise 0.”;
- GB::usage=” If use grain boundary put 1 in the Fracture energy file, otherwise 0.”;
- TS::usage=” If use Thermal Stress put 1 in the Fracture energy file, otherwise 0.”;
- ltemp
- lnew::usage=”lnew is a half length of new microcrack in the crack propagation.”;
- delta::usage=”It defines the distance between new added inclusions.”;
- l2ratio::usage=”It is the 1/e ratio, where e is the aspect ratio.”;
- ttest::usage=”Is the number of cracks that are being added to the main crack to predict crack propagation more accurately.”;
- inc::usage=””;
- naccuracy::usage=””;

Number of parameter in the list is $ntot-1$ or $ntot-(inclusionsparticipateinthecrack)$

1.8 README-ThermalExpansion

- ThermalExpansion0 = Thermal expansion coefficient of the matrix material
- ThermalExpansiontemp = list of thermal expansion coefficient of the inclusions
- TStart = Initial temperature
- TEnd= End temperature

1.9 README-COMPRESSION

COMPRESSION: In this file crack propagation from two ends is simulated. This can be used either for tension or expansion. The *ntot* inclusion is the one that propagates.

main-crack-oneDirection: In this file the main-crack-One path propagation from RHS is simulated. The *\ntot*” is the inclusion that propagates.

1.10 README-LinearSolve

2 List of variables and functions used in the code

geometry.m

1. n::usage =”number of harmonic terms”;
2. num1::usage =”Crack propagation criterion. Number 1, is the to search on the surface of inclusion for max
3. energy, number 2 uses SIFs.”;
4. num2::usage =”It determines which process has to be used to calculate SIF; 1 is the formula from MM, 2 is the average SIF over short distance.”;
5. ntot::usage =”total number of inclusions in the system”;
6. Chi0::usage =”Chi0=3-4Nu0 for plain strain and (3-Nu0)/(1+Nu0) for plane stress.”;
7. Nu0::usage =”Nu0 matrix poisson ratio”;
8. Mu0::usage =”Mu0 matrix shear modulus”;
9. Theta::usage =”angle of inclination for each inclusion [-90,90]”;
10. Thetaprim::usage =”angle of inclination for each inclusion [0,360]”;
11. dd::usage =”2d is the inter-foci distance of an inclusion”;
12. Dq::usage =”2d is the real part of the inter-foci distance of an inclusion”;
13. dpq::usage =”dpq=dp+dq”;
14. Zeta0::usage =”Zeta0[p]=The matrix-inclusion inerface of the p particle”;
15. v0::usage =”v0=Exp[Zeta0]”;
16. Chi::usage =”Chi=3-4Nu”;
17. MuBar::usage =”relative shear modulus”;
18. Nu::usage =”Poisson ratio”;
19. E0::usage =”Matrix material Young’s Modulus in GPa”;
20. EQ::usage =”Inclusions Young’s Modulus in GPa”;
21. l1::usage =”l1=major semi - axes of the ellips”;

22. l2::usage =”l2=minor semi - axes of the ellips”;
23. MuQ::usage =”shear modulus”;
24. s11::usage =”s11 Farfield stress field”;
25. s12::usage =”s12 Farfield stress field”;
26. s22::usage =”s22 Farfield stress field”;
27. tetatemp::usage =”Inclusion inclination angle [-90,90]”;
28. tetatempprim::usage =”Inclusion inclination angle [0,360]”;
29. e::usage =”ellipse aspect ratio”;
30. l1temp::usage =”Read information about the inclusion from the input file.”;
31. l2temp::usage =”Read information about the inclusion from the input file.”;
32. NuQtemp::usage =”Read information about the inclusion from the input file.”;
33. MuQtemp::usage =”Read information about the inclusion from the input file.”;
34. zcenter::usage=” center point of new inclusions(cracks) in the global coordinate system”;
35. zcenter1::usage=” zcenter”;
36. zcenternewlist1=” center point of new inclusions(cracks) in the global coordinate system”;
37. G0::usage =”Fracture energy of host material.”;
38. GQ::usage =”Fracture energy of inclusions.”;
39. kQ::usage =”Surface perfectness of inclusions.”;
40. GintQ::usage =”Fracture energy of interface of the inclusions (G0*kQ[i]).”;
41. GGB::usage =”Fracture energy of the grain boundaries.”;
42. vertexList::usage =””;
43. BE::usage=” If use finite boundary put 1 in the Fracture energy file, otherwise 0.”;

44. GB::usage=" If use grain boundary put 1 in the Fracture energy file, otherwise 0.";

45. TS::usage=" If use Thermal Stress put 1 in the Fracture energy file, otherwise 0.";

46. EndPoint::usage = "EndPoint[p]= EndPoint of the inclusion";

47. StartPoint::usage = "StartPoint[p]= StartPoint of the inclusion";

48. lnew1::usage="lnew1/2 is a vertical distance from the surface of the inclusion at eta0 angle.";

49. delta::usage="It defines the distance between new added inclusions.";

50. l2ratio::usage="It is the 1/e ratio, where e is the aspect ratio.";

51. lnew::usage="lnew is a half length of new microcrack in the crack propagation.";

52. ttest::usage="Is the number of cracks that are being added to the main crack to predict crack propagation more accuratly.";

53. inc::usage="";

54. naccuracy::usage="";

55. lnewtest::usage="l2test[deltat,l1t]";

56. LNEW::usage="LNEW[i]";

57. LNEW1::usage="LNEW1";

58. ChangeLNEW::usage="ChangeLNEW[ninitial1]";

59. ChangeLNEW1::usage="ChangeLNEW1[deltat,lt]";

60. Changelnewsize::usage=" Changelnewsize[lnewt,deltat]";

61. Deltatest::usage="Deltatest[l2,l1t]";

62. DELTANEW::usage="DELTANEW[initial1]";

63. DELTANEW1::usage="DELTANEW[initial1]";

64. ThermalExpansion0::usage="ThermalExpansion0= Matrix material thermal expansion 1/K";

65. ThermalExpansionQ::usage="ThermalExpansionQ= Inclusions' thermal expansion 1/K";

66. ThermalExpansiontemp::usage="An array of Inclusions' thermal expansion 1/K";

67. TStart::usage="Initial temperature! (K)";

68. TEnd::usage="End temperature! (K) ";

69. FractureEnergyBC::usage="FractureEnergyBC[BE1,GB1]";

70. nChange::usage="nChange[naccuracy]";

71. FilePath::usage ="Please choose directory of the package.";

72. OutputFile::usage ="Path to Output file";

73. InputFile::usage ="Path to input file";

74. FractureEnergyOutputFile::usage ="Path to Fractureenergy file in output folder";

75. FractureEnergyInputFile::usage ="Path to Fractureenergy file in input folder";

76. ThermalExpansionFile::usage ="Path to ThermalExpansion file in output folder"; (*mFilesPath::usage ="Path to mFiles folder.";*)