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# Simulations on Statistical Representations of Polycrystals using FRANC2D/L

*Polycrystal User's Guide*

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Erin Iesulauro and Ketan Dohdia  
Cornell University • Ithaca, New York

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## Introduction

After examining the microstructure of the AA 7075-T6, a meso-scale representation was created on which to perform simulations and to study the microstructural influences on crack initiation. The process of creating a meso-scale model with discrete grains represented was broken down into three stages: creating a grain geometry, determination of material model and properties for the grains, and determination of how to represent the grain boundaries to allow the initiation of cracks.

## Outline of Procedure

### Grain Geometry

The representation of the grain geometry could either be done to match a single observed polycrystal sample or to represent the average geometry seen over many samples. It was decided to represent the geometry in an average sense. The polycrystal samples generated statistically match observation in terms of quantities such as average grain size and aspect ratio. However, samples won't exactly match any observed geometry. For this work, the Voronoi tessellation was chosen as the method by which to create the grain geometries.

### Voronoi Tessellation

Voronoi tessellation begins from a random distribution of nuclei. Lines are generated connecting a nucleus to its nearest neighbors. These lines are then perpendicularly bisected to create the edges of a polygon. Each nucleus then defines a polygon within which all points are closer to the nucleus than to any other. This process best represents the initial forming of the grains from dendrite sites within a melt with isotropic growth rates [Arawde].

This particular choice represents the initial polycrystal structure or annealed structure well. However, Voronoi tessellations do not capture the distortion of the grains due to processing such as rolling. Since this work was done in 2D it was determined that this would be a good tessellation with which to test modeling choices and software capabilities. Ongoing work is looking at modifications to the Voronoi tessellation as well as other tessellation methods that will better represent the rolled grain structure.

Current modeling has been expanded to consider the discrete modeling of sub-grain sized particles. Particles well below the size of the grains are considered to be smeared out and represented through the grain material properties.

## Grain Material

Once the geometry is in place material properties are assigned to each grain. Current material model options include elastic, isotropic; elastic, orthotropic; isotropic, elastic-plastic; and orthotropic, elastic-plastic. Details concerning the plasticity implementation can be found in James. See the FRANC2D/L User's Guide for the necessary parameters. For the chosen material model each grain is assigned values of the appropriate parameters.

## Grain Boundaries

In a polycrystal there are many mechanisms that can lead to the initiation of micro-cracks. For example, fatigue leads to the formation of slip bands within grains, which can lead to shear cracks. Also, a corrosive environment can lead to the failure of grain boundaries due to oxygen embrittlement. The simulations conducted focus on grain boundary decohesion as the primary source of localized damage. To allow decohesion to occur naturally grain boundaries were modeled using cohesive zone models. The following discusses the theory and implementation of cohesive zone models.

### Grain Boundary Property Assignment

Grain boundaries naturally arise in polycrystals due to the lattice mismatch between adjacent grains. This region of disordered atoms acts differently than the regular lattices of the adjacent grains. Therefore, we describe the grain boundary with its own constitutive relationship, separate from the bulk grain material. A cohesive zone model has been chosen for this purpose to describe the strength and toughness of the grain boundaries. The cohesive zone model also serves as a criterion for initiation of intergranular cracks. The grain boundaries are allowed to decohere after reaching a critical normal, shear, or combined transmitted traction, thus gradually initiating a crack. Once a critical opening is reached a true crack has formed. An advantage of using such a model is that initial cracks are not arbitrarily introduced at the beginning of a simulation. Instead, cracks naturally occur due to the heterogeneous stress field throughout the sample caused by the geometry and variations in properties.

### Cohesive Zone Model

In theory, the stress at a crack tip goes to infinity creating a stress singularity. However, in practice materials, especially metals, have a yield stress at which they begin to deform plastically negating the singularity. This leads to the area around the crack tip called the crack tip plastic zone. The stress in the plastic zone can only reach the yield stress. The additional stress due to the singularity must still be carried by the material. Several methods have been developed to determine the extent of the plastic zone and account for

the stress beyond the yield stress. These include the Irwin's plastic zone correction and the strip yield models developed first by Dugdale and Barenblatt .

Dugdale considered a fictitious crack tip a distance  $\rho$  ahead of the actual crack tip. The fictitious tip carries a compressive force equal to the yield stress that tends to close the crack. An application of this approach by Hillerborg is the fictitious crack model or the cohesive zone model. The cohesive zone model (CZM) assumes that the compressive force applied in the plastic zone follows a traction-displacement relationship. It is also assumed that this traction-displacement behavior can be considered a material property [Broek][Anderson].

In the present case the damage represented by the strain softening portion of the CZM is used to describe the decohesion of the grain boundaries leading to crack initiation. Also, the area under the curve represents the critical energy release rate,  $G_c$ , to initiate a crack. The implementations available in FRANC2D/L [James], includes independent normal and shear cohesive models as well as a coupled model added for this work. The normal and shear models evaluate the transmitted traction independently of each other. In other words, the transmitted normal does not influence the amount of shear and vice versa. The coupled cohesive zone model (CCZM) implemented was adapted from a model developed by Tvergaard and Hutchinson, where the normal and shear components of the traction and displacement are combined into single measures,  $\tau$  and  $\lambda$ , respectively (Figure 1), so that responses are coupled.

### Coupled Cohesive Zone Model

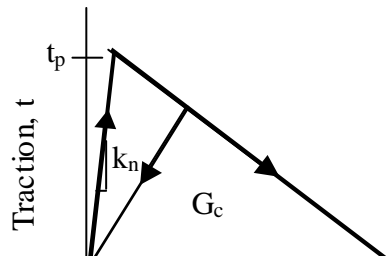


Figure 1: Coupled cohesive zone model

With the segregated models implemented problems can arise under mixed-mode loading. For example, since the shear and normal operate independently it is possible for shear forces to be transmitted across an interface while no normal traction is being transmitted due to large opening. This of course is physically incorrect. Since mixed mode loading is to be expected in polycrystal samples due to inclined grain boundaries the following coupled cohesive zone model (CCZM) was implemented.

The CCZM begins from a traction potential,  $\Phi$ .

$$\Phi(\delta_n, \delta_t) = \delta_n^c \int_{\lambda} t(\lambda') d\lambda' \quad \text{Eqn. 1}$$

$\Phi$  is a function of the relative normal,  $\delta_n$ , and tangential,  $\delta_t$ , displacements between the faces of the grain boundary.  $\lambda$  is a non-dimensional separation measure for the relative opening and sliding defined by Eqn. 2. The opening and sliding displacements are normalized to the relative critical displacement values,  $\delta_n^c$  and  $\delta_t^c$ , at which the separation is considered a true crack in pure Mode I and pure Mode II. When the value of  $\lambda$  reaches 1 this indicates the complete decohesion of the grain boundary and the formation of a true crack.

$$\lambda = \left[ \left( \frac{\delta_n}{\delta_n^c} \right)^2 + \left( \frac{\delta_t}{\delta_t^c} \right)^2 \right]^{1/2} \quad \text{Eqn. 2}$$

For a given relative displacement between two grains the combined traction,  $\tau$ , transmitted across the grain boundary can be determined from the CCZM. The combined traction can then be decomposed into normal,  $T_n$ , and shear,  $T_t$ , components by differentiating  $\Phi$  with respect to  $\delta_n$  and  $\delta_t$  according to Eqn. 3 and Eqn. 4 respectively.

$$T_n = \frac{\partial \Phi}{\partial \delta_n} = \frac{t(\lambda) \delta_n}{\lambda \delta_n^c} \quad \text{Eqn. 3}$$

$$T_t = \frac{\partial \Phi}{\partial \delta_t} = \frac{t(\lambda) \delta_n^c \delta_t}{\lambda \delta_t^c \delta_t^c} \quad \text{Eqn. 4}$$

The CCZM parameters have the following physical implications. The initial stiffness,  $k_n$ , represents the elastic response of the grain boundary. Since the grain boundaries are considered to be stiffer than the bulk grain material  $k_n$  is set to a high value. The coupled value of  $t_p$  relates to the peak normal strength,  $t_p^n$ , and peak shear strength,  $t_p^t$ , according to Eqn. 5 and Eqn. 6 respectively. Whether plane stress or plane strain is assumed will vary the value of the coupled peak traction,  $t_p$ , relative to the bulk yield stress. For plain strain  $t_p$  is considered to be three to five times the yield stress. For plane stress the value is only one to one and a half time the yield stress. For the parametric study the value of  $t_p$  is set to observe the influence of the relative values. After the peak traction is reached atomic bonds begin to break allowing the faces to separate. This portion is considered the softening of the grain boundary. At a specific distance the opposing face no longer exerts attractive forces on each other resulting in a true crack. This corresponds to  $\lambda = 1$ .

$$t_p = T_p^n \quad \text{Eqn. 5}$$

$$t_p = \delta_n^c T_p^t \quad \text{Eqn. 6}$$

### **Unloading of the Coupled Cohesive Zone Model**

Since cyclic loading conditions will be used, the unloading of the CCZM must be considered and implemented. Two possible unloading paths considered were unloading according to the initial stiffness and unloading back to the origin. Both physical

implications of the unloading paths and numerical difficulties were considered before choosing to unload to the origin.

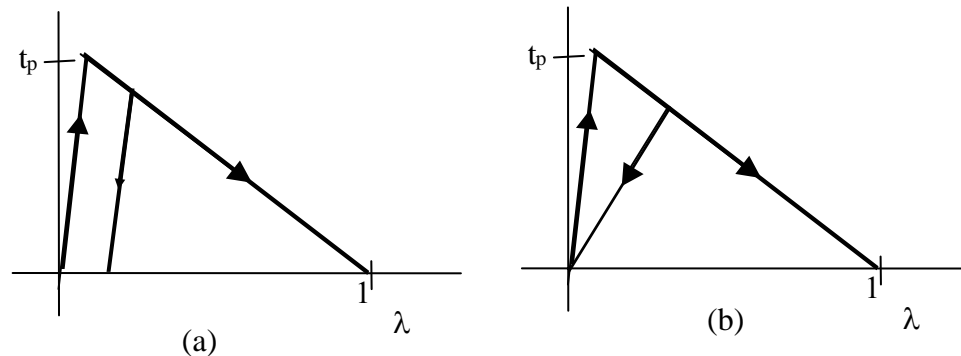


Figure 2: (a) Unloading according to the initial stiffness. (b) Unloading back to the origin

Unloading according to the initial stiffness allows for plastic deformation in the grain boundary to occur. Once the interface has returned to zero traction the displacement is not necessarily zero. This reflects such theories as crack closure. However, this approach causes implementation problems. When the FRANC2D/L software calculates the stiffness matrix for the model a tangent stiffness is determined for each element. For the interface elements the secant stiffness is calculated instead. The solution technique used requires the stiffness matrix to be positive definite. Therefore the negative slope of the softening portion of the curve is not acceptable. To compensate for this the secant stiffness is calculated instead, which still captures the softening of the stiffness matrix. Keeping this in mind, it follows that by unloading according to the initial stiffness would result in an increase in stiffness of the interface upon unloading and reloading.

Unloading back to the origin does result in a fully closed interface. However, the interface instead sees damage through maintaining a lower stiffness value upon reloading. This also removes several difficulties that would be experienced in implementation. For this reason unloading back to the origin was implemented.

## **Interface Elements**

A convenient method for implementing the CZMs is through zero thickness interface or joint elements. The 6 noded interface element (Figure 3) implemented here creates traction forces as a function of the displacement prescribed by the CZM. The displaced location of the centerline of the element is determined from the nodal positions. From this the relative displacements of node pairs are determined and interpolated to the Gauss integration points. At each of the integration points the traction is then computed from the CZM specified and integrated to determine the work equivalent nodal loads. The stiffness can also be determined from the CZM based on the relative displacement [Wawryznek][Bittencourt]. A tutorial for using interface elements in FRANC2D/L

simulations is included in Appendix A of Iesulauro or in the FRANC2D/L User's Guide version 2.0.

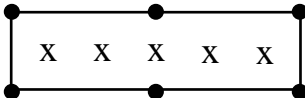


Figure 3: 6-noded interface element and location of intergration points



# Creating Statistical Samples of Polycrystals for FRANC2D/L

The \*.inp file for Franc2D/L contains mesh information as well as material definitions and assignments to each element. Traditionally creating an \*.inp is done using CASCA. This is an independent modeling and meshing program. A description of this tool is available in the FRANC2D and FRANC2D/L Manuals.

The statistical creation of polycrystal models and the corresponding \*.inp however, is not done through CASCA. Instead a series of Matlab functions were created to statistically generate polycrystal geometries and distributions of particles and as well as distributions of material properties.

The follow outlines the steps for creating a polycrystal sample and the corresponding \*.inp file. The next section contains an tutorial including commands for creating a polycrystal sample.

## Grain Geometry

Grain geometries are determined using Voronoi tessellation as described previously. The process of creating the tessellation has been compiled into a single Matlab script, *DM\_tess*.

*DM\_tess('jobname',dim,num,seed,seed)*

'*jobname*' is a string indicating the name to be used for the output file. *DM\_tess* calls a fortran program Vor.f that creates the tessellation. This program produces a square sample. *Dim* is the dimension of the square to be tessellated. Vor.f requires either the number of grains to be created or the average grain size. *DM\_tess* is currently set to accept the number of grains, *num*. FRANC2D/L is capable of reading up to 500 material definitions. This includes grain materials as well as cohesive zone model definitions. This should be taken into account when determining the number of grains to create. Finally, 2 random number seeds are needed.

The output is the file *jobname.tess*. This contains the tessellation information. To view the tessellation use *DM\_plottess('jobname')*. There are also several intermediate files that are generated but are not necessary for future steps.

## Particle Insertion

Polycrystal samples can be created with or without the inclusion of particles. The following describes the process for inserting particles distributed throughout the polycrystal. If you do not wish to have particles present skip to the next section.

***DM\_ParticleList('jobname',n\_parts,n\_sides,ratio,threshold,subdivide\_ratio\_max,subdivide\_ratio\_min,seed)***

Again ***jobname*** is used for reading the \*.tess file created and for naming output files. ***N\_parts*** is the number of particles you wish to have. Each particle will be represented as a polygon, ***N\_sides*** is the number of sides to be used for the polygons. ***Ratio*** determines the relative size of the particles to the size of the grains. The rest of the variables are used for determining overlap of particles and grain boundaries and for preparing the particles to be meshed. ***Threshold*** is the minimum distance allowed between a particle and a grain boundary. If a particle is closer than the value of threshold then the particle is moved such that it will touch the grain boundary. This value is also used to determine the minimum distance between particles. If particles are too close they will be joined. The subdivide\_ratios are used for subdividing the particle edges for meshing. The subdivisions must be between the min and max\*longest edge. Finally a random number seed is also needed.

The output is ***jobname.sub***, a list of subdivision of particle boundaries for meshing, and ***jobname.par***, a list of the particles. When the function concludes it will display the tessellation with the particles in a Matlab figure window.

## **Meshing**

Once the polycrystal geometry has been defined and the particles defined and placed the model can be meshed. Meshing routines are called from ***DM\_mshtess***. ***DM\_mshtess*** uses the \*.tess and \*.par files to generate the mesh along with ***properties.txt***, ***partprop.txt***, ***betalist.txt***, and ***hardcurve.txt***. ***Properties.txt*** and ***partprop.txt*** define the distribution of properties to be assigned to the grains and particles respectively. This is described further below. ***Betalist.txt*** is a file listing the distributions of material angles to be used for assigning lattice angles to the grains. ***Hardcurve.txt*** is used to define hardening curves for von Mises materials. Currently the particles are modeled as elastic, isotropic. The command is as follows.

***DM\_mshtess('jobname',mat,dim,nseed,nseed2,subdiv\_ratio)***

Again '***jobname***' is the name used to create previous output files that ***DM\_mshtess*** will call. If isotropic grains are being used this file is ignored. ***Mat*** is an integer that indicates the material model to assign to the grains (1-Elastic-Isotropic, 2 – Elastic-Orthotropic, 3 – von Mises, 4 – Hill). The dimension of the sample is again requested in ***dim***. Next 2 random number seeds are given. Finally, if a subdivide file (\*.sub) is not

provided the mesh generator using the single value specified by *subdiv\_ratio*. This determines the density of the mesh.

### **Assigning Grain Material Properties**

The meshing step also assigns material numbers to each element. The material numbers refer to a defined material model. For each sample a material model is chosen to describe the grain material. To add statistical variation for the given material model a different set of parameters can be assigned to each grain throughout the sample.

For each parameter in the material model a mean value and range are read from the *properties.txt* file. These values define a uniform distribution of values for the parameter. Matlab then creates a material definition by selecting values from the uniform distribution for each parameter. The format of the file is as follows.

```
E1: mean range std deviation
E2: mean range
E3: mean range
Poisson's Ratio: v1 v2 v3
Thickness
Density
KIC: mean range std deviation \\
KIC_inf
σy1d1: mean range
σy1d2: mean range
σy1d3: mean range
```

If particular values are unnecessary for the chosen model 0's can be entered as placeholders.

If von Mises, elastic-plastic material properties are desired for the grains *hardcurve.txt* can be used to define a uniform distribution of hardening curves. The file consists of the yield stress, ultimate stress and a range of variation.

Finally, in the case of orthotropic materials, *betalist.txt* is necessary. This file contains a distribution of angles from which each grain is assigned a lattice orientation. The angle assigned is the angle measured counter-clock wise from the global X-axis to the primary axis of the lattice. In the Hill case, this is the primary yield stress direction.

### **Assigning Particle Material Properties**

A similar process is followed for defining material models for the particles and assigning material numbers to the elements within each particle. The particle properties are taken from the file *partprop.txt*. Currently particles are defined as elastic, isotropic so the file format is as follows.

```
E1: mean range std deviation
```

```

Possion's Ratio:  $\nu_1 \nu_2 \nu_3$ 
Thickness
Density
KIC: mean range std deviation \

```

The meshing processing creates several intermediate files. These files include *tess.out* and *particle.out*. The final output is an \*.inp file. This file can be read by FRANC2D/L.

## Defining Cohesive Zone Models

This \*.inp file created at this point is readable by FRANC2D/L; however, it does not contain any information concerning the grain boundaries or particle-grain interfaces. As discussed previously these responses are determined by CCZMs. This information can be entered from within FRANC2D/L. If different parameters are used for each grain boundary it is more efficient to define the models before hand. This is done through two additional Matlab scripts: *DM\_MultiCZM1* and *DM\_ParticletCZM*.

### *DM\_MultiCZM1('jobname',beta)*

*DM\_MultiCZM1* appends *jobname.inp* with parameters defining one more more cohesive zone models corresponding to ranges of angles of misorientation between grains. To determine the ranges of properties to be assigned by *DM\_multiCZM1* the file must be altered to reflect the values. *Beta* is the angle range for which each CZM to be defined will be good for. For example, if you want to use 1 CZM for all grain boundaries  $\Delta = 360$ . If instead  $\Delta = 5$ , then the first CZM will be valid for grain boundaries with a misorientation angel between 0 and 5 degrees and then next for 6 to 10 degrees and so forth.

### *DM\_ParticleCZM('jobname')*

*DM\_ParticleCZM* again appends *jobname.inp* with parameters defining a CZM. This cohesive zone defines the response of the particle-grain interface. The properties are read from the file *Part\_czm.txt*.

## Input \*.inp File Format

The steps outlined above result in an .inp input file for FRANC2D/L. The file includes mesh information as well as material definition and assignments, and cohesive zone models definitions. The following is an example .inp file for the 16-element block shown in Figure 4.

```

65 16 1 1
 1 2.90E+04 2.50E-01 1.00E+00 1.00E+00 1.00E+00 0.00E+00
   0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 1 1 6 1 53 52 51 2 9 7
 2 1 9 2 51 50 49 3 12 10

```

```

3   1  12   3  49  48  62  61  60  13
4   1  42   4   6   5  16  14  44  43
5   1  16   5   6   7   9   8  19  17
6   1  19   8   9  10  12  11  22  20
7   1  22  11  12  13  60  59  58  23
8   1  44  14  16  15  26  24  46  45
9   1  26  15  16  17  19  18  29  27
10  1  29  18  19  20  22  21  32  30
11  1  32  21  22  23  58  57  56  33
12  1  46  24  26  25  35  34  64  47
13  1  35  25  26  27  29  28  37  36
14  1  37  28  29  30  32  31  39  38
15  1  39  31  32  33  56  55  65  40
16  1   6   4  42  41  63  54  53   1
1   1.500000E+00  1.750000E+00
2   1.000000E+00  1.750000E+00
3   5.000000E-01  1.750000E+00
4   1.750000E+00  1.500000E+00
5   1.500000E+00  1.250000E+00
6   1.500000E+00  1.500000E+00
7   1.250000E+00  1.500000E+00
8   1.000000E+00  1.250000E+00
9   1.000000E+00  1.500000E+00
10  7.500000E-01  1.500000E+00
11  5.000000E-01  1.250000E+00
12  5.000000E-01  1.500000E+00
13  2.500000E-01  1.500000E+00
14  1.750000E+00  1.000000E+00
15  1.500000E+00  7.500000E-01
16  1.500000E+00  1.000000E+00
17  1.250000E+00  1.000000E+00
18  1.000000E+00  7.500000E-01
19  1.000000E+00  1.000000E+00
20  7.500000E-01  1.000000E+00
21  5.000000E-01  7.500000E-01
22  5.000000E-01  1.000000E+00
23  2.500000E-01  1.000000E+00
24  1.750000E+00  5.000000E-01
25  1.500000E+00  2.500000E-01
26  1.500000E+00  5.000000E-01
27  1.250000E+00  5.000000E-01
28  1.000000E+00  2.500000E-01
29  1.000000E+00  5.000000E-01
30  7.500000E-01  5.000000E-01
31  5.000000E-01  2.500000E-01
32  5.000000E-01  5.000000E-01
33  2.500000E-01  5.000000E-01
34  1.750000E+00  0.000000E+00
35  1.500000E+00  0.000000E+00
36  1.250000E+00  0.000000E+00
37  1.000000E+00  0.000000E+00
38  7.500000E-01  0.000000E+00
39  5.000000E-01  0.000000E+00
40  2.500000E-01  0.000000E+00
41  2.000000E+00  1.750000E+00
42  2.000000E+00  1.500000E+00
43  2.000000E+00  1.250000E+00
44  2.000000E+00  1.000000E+00
45  2.000000E+00  7.500000E-01
46  2.000000E+00  5.000000E-01
    
```

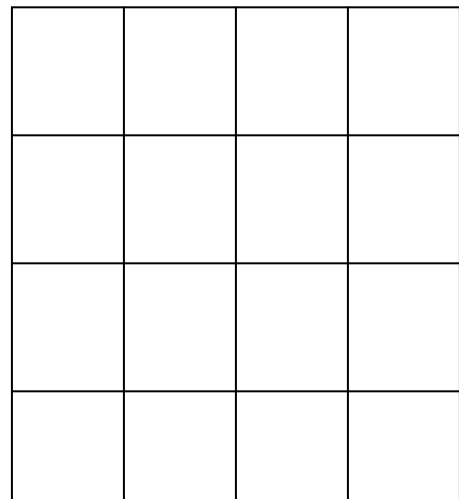


Figure 4: 16-element block

47	2.000000E+00	2.500000E-01
48	2.500000E-01	2.000000E+00
49	5.000000E-01	2.000000E+00
50	7.500000E-01	2.000000E+00
51	1.000000E+00	2.000000E+00
52	1.250000E+00	2.000000E+00
53	1.500000E+00	2.000000E+00
54	1.750000E+00	2.000000E+00
55	0.000000E+00	2.500000E-01
56	0.000000E+00	5.000000E-01
57	0.000000E+00	7.500000E-01
58	0.000000E+00	1.000000E+00
59	0.000000E+00	1.250000E+00
60	0.000000E+00	1.500000E+00
61	0.000000E+00	1.750000E+00
62	0.000000E+00	2.000000E+00
63	2.000000E+00	2.000000E+00
64	2.000000E+00	0.000000E+00
65	0.000000E+00	0.000000E+00

The first line includes the number of nodes, number of elements, number of material definitions, and the problem type.

This is followed by the material definitions. Materials are numbered according the order they are listed. Therefore material numbers are not explicitly listed in the .inp file. For each material definition the first number is the material model (1 – Isotropic, 2 – Orthotropic, 3 – von Mises, 4 – Hill). The following numbers are the parameters for the given model.

Next the element conductivities are listed. The element number is followed by the material definition assigned to that element and the nodes listed in *counterclockwise* order.

Next the nodes are listed. Each line contains the node number followed by the X and Y coordinates.

This would be the end of a typical FRANC2D/L input file. However, information concerning the von Mises materials and the cohesive zone models are appended to the end of the file.

The von Mises plasticity model implemented allows hardening to occur. Normally the hardening curve is defined after opening FRANC2D/L. However, with many materials defined this becomes inefficient. Therefore the definitions of these curves were appended to the .inp file following the text string 'HARDCURVE'. For each von Mises material defined several lines are appended. The first line indicates the number of points used to define the curve. Each subsequent line lists the X and Y coordinates of a point on the curve.

Next the coupled cohesive zone models for the grain boundaries are listed following the text string 'multiCZM'. Each coupled cohesive zone model is valid for a range of

misorientations measured across the grain boundary. The angle range is listed first followed by the model parameters.

Finally, the CCZM used to define the particle-grain interface is listed following the text string 'partCZM'. The format is the same as listed above. However the angle range is given as 0 360. Currently all particle-grain interfaces follow the same response so just one model is defined. The angle range is still list however for consistence and the ability to easily expand in the future.

# FRANC2D/L Example

## Building an Initial Geometry and Mesh

The polycrystal and mesh are generated from Matlab. First create the tessellation as follows.

*DM\_tess('jobname',dim,n,nseed)*

For this example the following input was used.

```
DM_tess('tutorial',0.5,100,5492)
```

Figure 4 shows the results from *DM\_tess*.

This is a simple example therefore particles were not placed in the polycrystal. Therefore, the next step is to mesh the tessellation, assign grain material properties, and define cohesive zone models.

The next step is to mesh the polycrystal sample and assign material properties to the grains. For this example the grains are elastic, isotropic. Therefore, only the *properties.txt* file is needed.

```
DM_mshtess('tutorial',1,0.5,268,542,.1)
```

For this example *hardcurve.txt*, *betalist.txt*, and *partprop.txt* were not used. The following are the input files *properties.txt*.

```
Properties.txt:  
72 2 1  
0 0  
0 0  
0.34 0.35 0.35  
1  
1.0  
0.00632 0.0 25  
10000000  
0 0  
0 0  
0 0
```



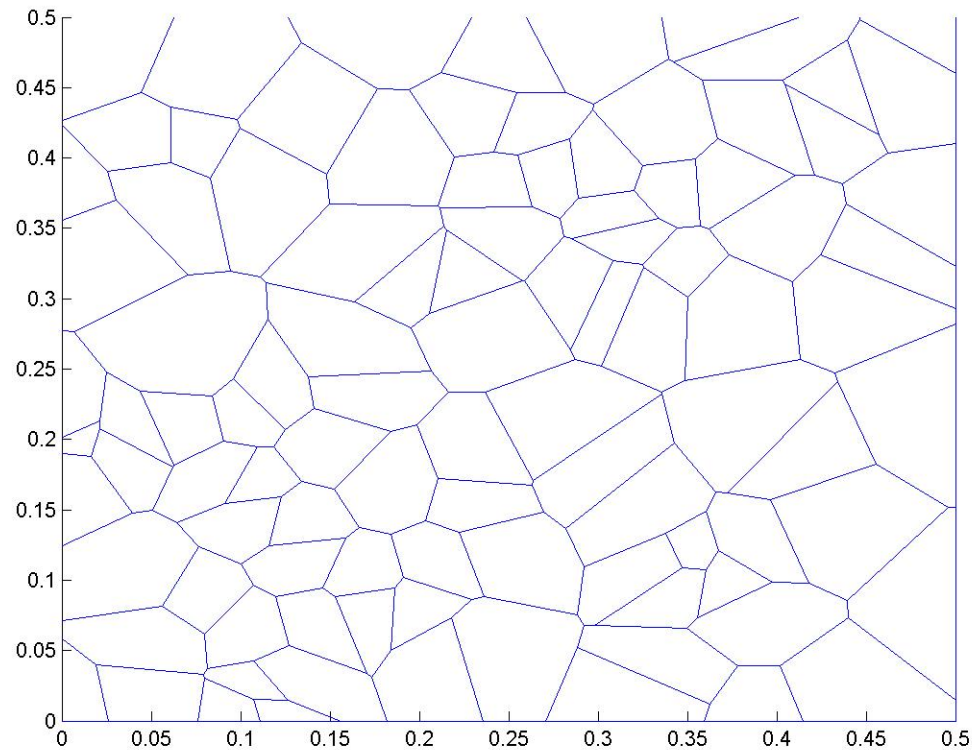


Figure 5: Matlab figure output from *DM\_tess*

Finally, the interface properties are assigned by the following statements. To simplify this example one CZM will be used for all of the grain boundaries. Therefore the angle inputted to *DM\_multiCZM1* will be 360.

```
DM_multiCZM1('tutorial',360)
```

## **Performing a FRANC2D/L Simulation**

Start FRANC2D/L with the \*.inp file created above. Due to the size of the model it may be necessary to start the program with extra memory allocated. That is done by calling the program as shown below. This example is small enough that this command is not needed. However, for slightly larger models it will be needed.

```
Franc2dl.exe -mem 25000000
```

Due to the size of the models it may take a moment for the file to be read. Once the model is read in there are still several pre-processing steps before the model is ready for analysis. It is important to follow the procedure in the order listed. Of most importance is that the interface elements must be placed before applying displacements to the model.

### ***Defining the Problem Type***

The problem type is specified under **PRE-PROCESS→PROBLEM TYPE** menu. Plain strain is preferred for these models. However, if the grains are defined as Hill materials then plane stress must be used.

### ***Boundary Conditions: Fixities***

Fixities are applied from the **PRE-PROCESS→FIXITY** menu. For this example the bottom edge is fixed in the Y-direction. Also the center node is fixed in the X-direction. The center node is determined by using **EL/NO INFO→NODE INFO** to determine which node is closest to the center.

### ***Inserting Interface Elements***

At this time, if you did not define an interface model to be used on the grain boundaries do so now. If this information was appended to the \*.inp file then proceed.

As described in the FRANC2D/L version 1.5 user's guide a feature has been added to automatically place interface elements along all interfaces. The feature can be assessed through the **PRE-PROCESS→MATERIAL** menu. Use the **-MAT+** button to move to any interface model. In the bottom menu will be the button **PLACE ALL INTS**. Click on this button. To determine that the interface elements have been placed turn on the interfaces using the **INTRFC: ON/OFF** button. The interfaces will appear white while the other element edges will be orange. If an interface element is present the corresponding material number will be next to the element. Occasionally this feature encounters problems. If the program does not return quickly then the function is stuck. At this point the best advice is to create a new mesh and possibly a new tessellation.

### ***Setting the Material Properties***

The grains were assigned material numbers during the meshing process. Therefore no other action is required here.

### ***Applied Displacements***

Finally the displacements are applied. Using loads is discouraged with polycrystal models since the analysis will likely become unstable.

Apply a unit displacement to the top edge of the model from the **PRE-PROCESS→APPLD DISP** menu.

### ***Perform Analysis***

Before performing the analysis be sure to save a restart file. This can be done before or after setting the control parameters. If there is not enough memory the solver will stop and the program will need to be restarted with more memory. Starting from a restart file will make this go quicker.

Even if the grains are defined to be elastic, the presence of the interface elements makes the analysis material non-linear. Therefore select the **ANALYSIS→MAT-NONLIN** option.

Select **CONTROL PARAM** to set up the analysis. The parameters will appear in the auxiliary window. Using the menu buttons set the option as follows.

```

Load Sub-Steps      :          10
Global Tolerance    :          0.1
Max Iterations:      200
Load Factor 1 :      0
Load Factor 2 :      0
Load Factor 3 :      0
Load Factor 4 :      0
Load Factor 5 :      0
Load Factor 6 :      0
Appld Dist Factor   :          0.1e-7
Accelerate Iter:     NONE
New Analysis :      YES
Current Step :      0
Final Step :          10
Save Frequency :      0
Print Frequency :     50
Increment Method :    FIXED
Anaylsis Mode :      INCREMENTAL
Autosave File :     jobname

```

Return from this menu. Select **ANALYZE ONE** to conduct the analysis. Do to the large number of degrees of freedom the initial set up before the solve actually begins can take a several minutes. The total solve time for example is about 5 minutes.

### ***Post-Processing***

Post-processing options are discussed in the FRANC2D/L User's Guide. The feature of note for this simulation is **POST-PROCESS→CONTOURS→STRAIN→INT SEPAR**. This shows the separation experienced by the interface elements. This can be useful for identifying elements that have started to decohere or that have fully decohered.

## Acknowledgments

Prof. Anthony Ingraffea (Cornell University) has focused on the goal of developing the ability to rapidly model discrete crack growth for about fifteen years. FRANC2D/L represents the work of several generations of students: Prof. Ingraffea modeled discrete crack growth by changing a mesh described by a deck of computer cards, Victor Sauoma modeled discrete crack growth on a Tektronix terminal, Walter Gerstle modeled crack growth on an Evans and Sutherland display, and finally, Paul Wawrzynek (Wash) used a workstation, started from scratch, and introduced robust data schemes to the engineers who had come before. Layering has been added by Sudhir Gondhalekar and Srinivas Krishnan at Kansas State University. Mark James is the most significant developer of the code at Kansas State. He has stabilized the code, added new features, maintained the multiple platform versions, and done all the work necessary to make the code a genuinely useable tool. In addition, he is extending FRANC2D/L to include elastic/plastic fracture. The approach is the crack tip opening angle method of Dr. Jim Newman, NASA. The port of GRA to Windows 95/NT was done by Brian Hardeman.

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