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Introduction of Simulating the Motion of Rigid Ellipsoidal Objects in Ductile Shear Zone Based on the Jeffery's Theory

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Rigid ellipsoidal objects (gravels and porphyroclasts) in ductile zone is an important factor to indicate the kinematics and dynamics. Jeffery's theory (Jeffery G, 1922), a quantitative research method, for the rotation of the rigid objects (no deformation) in the Newtonian fluid of the simple deformation field has been widely applied by geologists to the study of fabrics in rocks. The theory propose a way to build the coordinate system and describe the marker sharp, rotation angular velocity and flow field as well as the motion of the rigid in a quantitative way which affected by external force(Dazhi Jiang, 2007; Liu et al, 2015).

1 The coordinate system

The coordinate is the basement for the computer simulation and describing the attitude of the rigid objects in the ductile shear zone. According to the Jeffery's theory two coordinate systems were needed to describe the rotation path of the object.

The theory (Jeffery G, 1922) define the three semi-axes of the rigid ellipsoid ɑ1，ɑ2, and ɑ3. For the triaxial objects, ɑ1,ɑ2,ɑ3 represent the the long, intermediate, and the short semi-axes (ɑ1>ɑ2 >ɑ3) respectively. Right handed coordinate system (x'y'z') with x'-,y'-,and z'-axes parallel to the ɑ1,ɑ2,ɑ3 respectively. This coordinate system rotates with the rigid object in the fixed external coordinate system, xyz, in which the flow of the matrix fluid is defined(Fig. 1). The theory denote the vectors e1',e2',e3' parallel to x',y',z', respectively, and e1,e2,e3, parallel to x,y,z, and let the two coordinates share the same origin.

The theory define the *X* as a position vector in the xyz system and *X'* as the corresponding vector with the corresponding coordinates in x'y'z' system. *X* and *X'* could be related by a coordinate transformation tensor Q or its transpose Q^T:

$$\mathbf{X'} = \mathbf{QX} \qquad \mathbf{X} = \mathbf{Q^T X'} \tag{1}$$

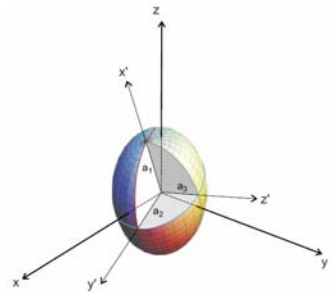

Fig. 1. Schematic diagram of the coordinate system (Jiang, 2007a)

2 Eulerian velocity gradient tensor

It is considered (Jeffery G,1922; Dazhi Jiang,2007) that the homogeneous flow field could be described by the Eulerian velocity gradient tensor L (in the xyz system) which can be decompose into two tensors, a strain rate tensor D and a vorticity tensor W according to:

L = D + W (2)

$$\mathbf{D} = \frac{1}{2}(\mathbf{L} + \mathbf{L^T}), \mathbf{W} = \frac{1}{2}(\mathbf{L} - \mathbf{L^T}) \tag{3}$$

The strain rate and the vorticity tensor also follows the tensor transformation which can be expressed in the x'y'z' system as following :

$$\mathbf{D'} = \mathbf{QDQ^T}, \quad \mathbf{W'} = \mathbf{QWQ^T} \tag{4}$$

3 Defining the shape and the angular velocity of a rigid ellipsoidal object

Jeffery(1992) define the shape of a rigid ellipsoidal object by three shape factors, B1,B2,B3 and let them follow the rules:

$$B_1 = \frac{(a_2^{\,2} - a_3^{\,2})}{(a_2^{\,2} + a_3^{\,2})} \quad B_2 = \frac{(a_3^{\,2} - a_1^{\,2})}{(a_3^{\,2} + a_1^{\,2})} \quad B_3 = \frac{(a_1^{\,2} - a_2^{\,2})}{(a_1^{\,2} + a_2^{\,2})} \tag{5}$$

It is reasonable to know that $B_3 = \frac{-(B_1 + B_2)}{(1 + B_1 B_2)}$ (6)

The rotation of the rigid ellipsoidal object is governed by the angular velocity which determined by the matrix flow, the shape of the rigid object and its instantaneous orientation in the flow.

The angular velocity could be expressed in the x’y’z’ system as follows:

$$\omega' = \begin{pmatrix} W'_{32} + B_1 \cdot D'_{23} \\ W'_{13} + B_2 \cdot D'_{13} \\ W'_{21} + B_3 \cdot D'_{12} \end{pmatrix} \tag{7}$$

The angular velocity, expressed in the xyz system, is:

$$\omega = \mathbf{Q}^{\mathbf{T}} \omega' \tag{8}$$

Then the rotation of the three principal axes of the rigid elllipsoid is defined by the time rate of the three unit vectors which parallel to their principal axes:

$$\frac{\mathrm{d}e'_i}{\mathrm{d}t} = \omega \times e'_i = \Theta e'_i \; (i = 1,2,3) \tag{9}$$

Θ is the tensor form of the angular velocity and for any vector $\mathbf{p}$, $\omega \times \mathbf{p} = \Theta \mathbf{p}$ (10)

4 Modeling the rotation of the single rigid ellipsoidal objects

By using the Runge-Kutta fourth-order method (Jeffery G, 1995) for Eq.(9) Leads to:

$$\begin{aligned} k_1 &= \delta t \Theta(t_n) e'_i(t_n) \\ k_2 &= \delta t \Theta(t_n + \frac{\delta t}{2})(e'_i(t_n) + \frac{1}{2} k_1) \\ k_3 &= \delta t \Theta(t_n + \frac{\delta t}{2})(e'_i(t_n) + \frac{1}{2} k_2) \\ k_4 &= \delta t \Theta(t_n + \frac{\delta t}{2})(e'_i(t_n) + \frac{1}{2} k_3) \\ e'_i(t_{n+1}) &\approx e'_i(t_n) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \quad (i = 1,2,3) \end{aligned} \tag{11}$$

δt is a small time increment, once the shape of the object and the external flow are known, the $\Theta(t_n)$ in the Eq(11) can be calculated. By using the Euler approximation(Dazhi Jiang, 2007) we can see that

$$\begin{aligned} \eta_i(t_n + \frac{\delta t}{2}) &\approx \eta_i(t_n) + \frac{\delta t}{2} \Theta(t_n) \eta_i(t_n) \\ \eta_i(t_n + \delta t) &\approx \eta_i(t_n) + \delta t \Theta(t_n) \eta_i(t_n) \end{aligned} \tag{12}$$

If we obtain the object orientation at $t_n + (\frac{\delta t}{2})$ and at $t_n + \delta t$.

As a result, with Eq(11), this leads to the new orientation $e'_i(t_{n+1})$ of the object after a time increment δt. Continuing with this iterative procedure, one tracks the rotation path of the object from its initial orientation to its final orientation would be gained(Dazhi Jiang, 2007).