Ice fabric development with a new fabric evolution model

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ABSTRACT. Ice crystal orientation fabric has a strong influence on ice flow due to the plastic anisotropy of ice. The evolution of crystal fabric is driven by strain-induced grain rotation, as well as recrystallization. Most fabric-evolution models ignore many of the physical processes involved, or are valid only for highly parameterized fabrics. In this paper, we outline a new fabric model that treats a variety of processes affecting fabric development, and is suitable for inclusion in flow models. The model is checked against thin-section data from the WAIS divide core. In addition, the model shows that that a large proportion of the observed variability in thin section samples is likely to be effectively stochastic in nature.

INTRODUCTION

An individual ice crystal has an anisotropic creep response, deforming most easily in shear parallel to the crystal basal plane. Plastic deformation of an ice polycrystal depends on the orientations of its constituent grains (Azuma, 1994). A polycrystal that is initially isotropic will develop a lattice-preferred orientation in response to applied strain, thus causing it to have a bulk anisotropic response. The development of a preferred orientation is guided primarily by intracrystalline slip. Due to interference between grains, there is a tendency for the c-axes to rotate away from the directions of principal extensional strain (Azuma and Goto-Azuma, 1996). Several other processes are also important to fabric development. Normal grain growth occurs as smaller grains are consumed by larger grains due to surface energy. In addition, near the melting point, migration recrystallization allows the nucleation of new, strain-free grains. These new grains grow rapidly at the expense of older grains with high strain energy (Duval and Castelnau, 1995). Polygonization is another recrystallization process in which dislocations in a highly strained grain arrange into a subgrain boundary, eventually producing two grains as the misalignment increases (Alley and others, 1997). Although the grains typically are misaligned by only a few degrees, this does have the effect of preventing the orientation distribution function from attaining a sharp maximum, as well as limiting grain sizes.

In order to model fabric development, a homogenization scheme must be used in order to relate the macroscopic stress and strain rate experienced by the polycrystal to the state experienced by individual grains. The two possible end members are the Taylor-Bishop-Hill (homogeneous strain) (Taylor, 1938) and the Sachs (homogeneous stress) (Sachs, 1928) assumptions. For many materials such as metals with several active slip systems, homogeneous strain turns out to be a good assumption. It has the advantage of maintaining spatial compatibility in between grains, in assuming that hard-oriented grains receive correspondingly more stress in order to produce the same strain as soft grains. For ice, in which basal dislocation glide is by far the easiest slip system, homogeneous stress is a better assumption (Thorsteinsson, 2002). The actual situation is intermediate, with softer-oriented grains receiving more strain less stress. Grain compatibility is maintained through intercrystalline slip, and shear on basal and non-basal slip systems. Molinari and others (1987) developed the viscoplastic self-consistent homogenization (VPSC) model. Each individual grain is represented as an inclusion in a homogeneous equivalent medium representative of the bulk polycrystal properties. This can allow for a compromise between the homogeneous stress and homogeneous strain assumptions. The VPSC model has been used for ice by several investigators (e.g. Gillet-Chaulet and others (2005), Castelnau and others (1997)). Azuma and Goto-Azuma (1996) used a conceptually similar scheme in which stress over the polycrystal is partitioned by the resolved shear stress on the basal plane of each individual crystal. Thorsteinsson (2002) took a similar approach using the assumption of a polycrystal with cube-like topology, with each grain having six neighboring grains. The velocity gradient on an individual crystal was adjusted by a softness parameter,

$$\epsilon^c = \frac{1}{\gamma + 6\mu} \left(\gamma T_0 + \mu \sum_{i=1}^{6} \frac{T_i}{T_0} \right) \tag{1}$$

,

where T_i is the resolved shear stress of grain i, T_0 is the resolved shear stress of the central grain, and γ and μ adjust the relative contributions of the central grain and the six nearest neighbors. This has the effect of making a soft (high resolved shear stress) grain surround by hard (low resolved shear stress) grains harder, and vice-versa.

In this paper, we outline a general fabric-evolution model, using discrete grains rather than a continuous distribution to represent the polycrystal. Each grain possesses various physical properties such as radius and accumulated strain. In addition, each grain has several neighboring grains, with which it interacts. This is somewhat similar to the approach taken by Thorsteinsson (2002) and by Kennedy and others (2013) to account for nearest-neighbor interactions. However, the previous works assumed each grain has 6 neighbors, whereas this model allows for more or fewer neighbors. Unlike previous discrete models, this model maintains mass balance in the polycrystal. Grains grow only at the expense of neighboring grains, as opposed to assuming a parabolic growth-law (e.g. Gow (1969)). Recrystallization also obeys mass balance, with the nucleated grain removing mass from its neighbors. Polygonization likewise is mass-conservative, with a grain splitting its volume in half.

Increases in average grain size can occur only by the disappearance of some grains. To allow this, the model has explicit connectivity between grains to represent spatial information. While ice fabric evolution is physically deterministic, it depends highly on effectively unobservable properties such as dislocation density distributions, inclusions, impurity content, and other factors. Therefore, treating the limited modeled physics as being deterministic is a stronger assumption that allowing for fabric development to be stochastic. To this end, recrystallization and grain rotation are stochastic.

MODEL FORMULATION

Grain rotation

The most important process governing the formation of crystal fabrics is deformation-induced grain rotation. Grain rotation is described using a Jefferys-Type equation (Azuma, 1994). Assuming homogeneous stress between grains, and assuming deformation solely due to basal glide, we have:

$$\dot{c}_i = W_{ij}c_j + \zeta D_{ij}^g c_j + c_i c_j c_k D_{jk}^g, \tag{2}$$

where c_i is the unit vector in the direction of the c-axis. D_{ij}^g and W_{ij} are, respectively, the local strain rate tensor of the grain, and the spin tensor in the vicinity of the polycrystal. Since slip is assumed to only occur on the basal plane, there is no contribution of local grain deformation to c-axis rotation. ζ is a softness paramter which allows for nearest neighbor interaction by modifying the viscosity of individual grains.

This relates the macroscopic velocity-gradient to the rate of change of orientation of each crystal. Commonly, a tensor-closure approximation of the Jefferys equation(**?**) is used to describe the evolution of a continuous ODF, rather than a discrete ODF as we use here. The continuous ODF is approximated by orientation tensors of even order. Orientation distribution functions can be decomposed into an orthogonal expansion using even-order orientation tensors $boldsymbola^{(2n)}$, which are formed by averaging the $(2n)^{th}$ order dyadic products of c over the orientation distribution function. For example, $a^2 = <c \otimes c>$. This is equivalent to a spherical harmonic expansion. Orientation tensors beyond sixth order are usually neglected. Rather than modeling the evolution of each individual fiber, instead one solves a closure approximation of Jefferys equation for the symmetric elements of the orientation tensors. Gillet-Chaulet and others (2005) modeled the evolution of the second-order orientation tensor, $a^{(2)} = <c \otimes c>$. This equation requires the integration of six independent values of $a^{(2)}$. This approach is computationally efficient, and is ideal for inclusion in flow models. However, tensor closure approximations have several drawbacks. As only low-order orientation tensors are included, they do not allow for general ODFs, and most commonly assume an orthotropic ODF. As well, it can be difficult to include physics other than strain-induced grain rotation. By evolving each particle separately with Jeffery's equation, this model makes no assumptions about the form of the orientation distribution function, although it is more computationally intensive than closure-based approximations.

Nearest-neighbor stress-transfer

The softness parameter (adapted from **?**) allows stress to be transferred between a grain and its neighbors, depending on the effective strain rates of the grains. This is done by multiplying the viscosity tensor of each grain by a scalar factor ζ:

$$\zeta = \xi \left((1-\gamma)\sigma_0 + \gamma \sum_{i=1}^{n} \frac{A_i \sigma_i}{\sigma_0} \right) \tag{3}$$

where ϵ_0 and ϵ_i are the effective shear strain rates of the center grain and grain i, respectively. A_i is the normalized area fraction between the center grain and grain i. ξ is a scaling factor taken over the polycrystal to maintain self-consistency with the bulk velocity gradient. The effective strain rates of each grain depend on the homogenization procedure used. This is explained later.

Grain radius evolution

To track the rheological properties of a polycrystal, it is necessary to know the volume of each grain. Grain boundaries migrate in order to minimize energy from dislocations, grain-boundary energy, and other factors. To track the migration of boundaries over time, we must have an expression for the area of boundaries between grains.

Let g^i be an arbitrary interior grain. This grain has neighbors $g_1, ..., g_m$, with radii r_j. Now, the grain has an "unadjusted" surface area S_i, proportional to $r2$. The unadjusted surface that g^j shares with g_i is s_{ji}^u. This is assumed to be proportional to $r_i/(_j r_j)$. Now, for mass conservation, we must have that the adjusted areas $s_{ij} = s_{ji}$. To do this, we take $s_{ij} = \frac{1}{2}(s_{ij}^u + s_{ji}^u)$.

Normal Grain Growth

Normal grain growth is induced by a driving force related to the local mean curvature at the grain interface. Since grains in this model do not have a explicit shapes, we must make some assumptions. Taken over the entire grain boundary, the integral of the mean curvature over the boundary of the grain must always be at least 4π. This means that, for example, the grain having negative curvature at a boundary must "make up" that curvature elsewhere on its boundary. In a physical polycrystal, this imbalance would be accounted for by the boundaries of the polycrystal. Here, we assume that the curvature over the surface of each grain is normally distributed, with a average mean curvature inversely proportional to the radius. Let r_1 and r_2 be the radii of two neighboring grains. At the shared boundary, the curvature of one grain must be the negative of its neighbor. Then, assuming independence, the average mean curvature over the shared boundary is given by $\frac{1}{r_1} - \frac{1}{r_2}$. The

grain boundary velocity due to curvature is then,

$$\frac{dr_1}{dt} = K\left(\frac{1}{r_1} - \frac{1}{r_2}\right) \tag{4}$$

where K is an Arrhenius factor dependent on temperature, and r_1 and r_2 radii of the two grains. However, as a simplification, we take the curvature of the boundary to be the harmonic mean of the curvatures of the two surfaces.

RECRYSTALLIZATION AND POLYGONIZATION

Migration (dynamic) recrystallization is driven primarily by lower-strain-energy grains consuming higher-strain energy grains (Duval and Castelnau, 1995). At least at larger scales (after the initial nucleation), this reduction in strain energy can be incorporated into the driving force of grain boundary migration. A grain neighboring a more highly strained grain will advance into the highly strained grain. This is due to the more highly strained grain having higher dislocation density. The dislocations are annihilated by the advancing boundary.

The strain rates of individual grains are then determined from the bulk stress tensor and the anisotropic viscosity of the individual grain. Following Azuma and Goto-Azuma (1996), the model calculates the effective stress on each grain, which depends on the bulk stress and the orientation of each grain and its neighbors.

Polygonization is caused by dislocations organizing into dislocation walls in grains experiencing elastic strain (Duval and Castelnau, 1995). Lattice misalignment between the two subgrains increases as more dislocations pile up, eventually splitting the grain into two separate grains misaligned by up to several degrees. We use a similar approach to Thorsteinsson (2002). If the difference of the magnitude of the RSS on the basal plane and the applied stress exceeds a critical value, and the accumulated strain exceeds a critical value, the grain splits into two equal portions. The angle of the split grain follows the Fisher distribution. For polygonization, it is not physically realistic to always assume that the polygonized grains rotate towards the direction of easy glide. For, if polygonization is very active, one would see groups of closely oriented grains lying linearly in the Schmidt plot, which is not seen in ice cores.

Model Validation

For a variety of flow situations, the model can reproduce characteristic fabrics such as single maxima, and large girdle fabrics. By incorporating recrystallization, double girdle fabrics and small girdles are produced. This is in qualitative agreement with typical ice-core fabric types. In ¡¡Figure 1¿¿, examples are given of several fabric types produced from different flow scenarios.

We validated the model by forcing it with from the West Antarctic Ice Sheet (WAIS) divide ice core. The flow near the WAIS divide ice-core site is dominated by uniaxial extension, with horizontal shear becoming important near the base. Dynamic recrystallization also occurs near the bed. The fabric in the core is a vertical girdle, which transitions to a vertical single maximum fabric near the bottom of the core. We validated the model by forcing it with data from the WAIS divide ice core, including temperature and a thinning function derived from the WDC06 chronology. This is then compared to thin-section data collected from the core (Donald Voigt, personal communication).

We assume that the thinning function follows the Nye rule CITATION. From the thinning function and the depth age relationship, we estimate vertical shear by assuming steady-state. Bulk stress is estimated from the properties of the polycrystal. In the coordinate system defined by the c-axis, an individual grain possesses a fourth-order viscosity tensor which can be represented as a diagonal 6×6 matrix in Voigt notation (where multiple elements in the tensor are mapped to the same matrix element by symmetries, Helnwein (2001)). The viscosity of the bulk polycrystal is then taken to be the volume-weighted average of each grain's viscosity tensor rotated into the macroscopic coordinate system. Then, the bulk stress tensor is found from the product of the viscosity tensor and the strain-rate tensor.

Thin Section Data

The ice-core thin-section data consist of 54 thin sections from depths of 140 meters to 3405 meters, and a corresponding age range of 480 years to $67,800$ B.P. There are several hundred grains in each thin section. The thin-section fabrics display oscillatory behavior. In figure 2, the smallest singular value of each sample is plotted. Some excursions are too large to be explained by sampling error.

The fabric model itself is conceptually a Lagrangian model tracking a single packet of grains as they are advected through the ice sheet over time, whereas each thin section possesses different initial conditions and physical properties. Thus, a this is expected to be a significant source of mismatch between between observed fabric and modeled fabric. The thin section at 140 m already shows significant development of a preferred orientation. This is consistent with the results of DiPrinzio and others (2005) at Siple Dome, where preferred orientations were observed in the firn as shallow as 22 m. In addition, at the Siple Dome site, recrystallization was found in some layers of shallow, cold ice. A similar process may contribute to the variability observed in the WAIS thin sections.

In addition to likely spatial inhomogeneities, there is sampling error due to small size of fabric samples. From modeling experiments, Thorsteinsson (2002) found that a sample size of around 5000 is needed for a small model variance, whereas the thin sections have sample sizes in the hundreds. However, sampling error is not enough to account for the large differences in fabric seen in the core (see next section)..

A common method to summarize a fabric with grain orientations X is to calculate eigenvalues and eigenvectors of the matrix formed by XX^T, or equivalently, calculate the singular values and vectors of the sample matrix. This can capture certain general features such as the strength of a single maximum fabric or a girdle fabric. However, it is unable to capture non-linear features of orientation distributions. For our analysis, we summarize fabrics using the "earth mover distance" (EMD). The

Fig. 1. Plot of the modeled smallest singular value of the modeled fabric versus that of the WAIS thin-section data. In the upper part of the core, there is a large girdle from extension in one horizontal axis, tending towards a single maximum as simple shear increases.
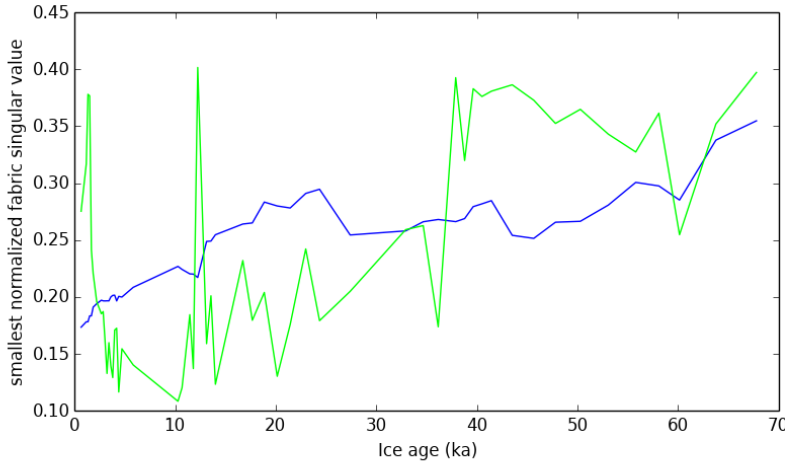

EMD between two point sets P_1 and P_2, with vectors of associated weights for each point W_1 and W_2, is given by the minimum work required to move the weights from points on P_1 to the points on P_2. In this case, we are transforming c-axis normal vectors from one observed fabric to another across the upper hemisphere. The work to move a weight w from a point x to a point y on the upper hemisphere is then given by wd, where d is the great-circle distance. This measure can detect changes in fabric which are not reflected in the fabric eigenvalues, such as the difference between a double girdle and a diffuse single girdle. In addition, it is a relatively robust measure, with qualitatively similar fabrics producing similar results. To model the "girdleness" and single-maximum strength of a fabric, we measure the EMD between the fabric and a perfect single maximum and a perfect girdle. That is, fabrics with c-axis orientations concentrated at only one point, in the case of a single maximum fabric, or along a plane, in the case of a girdle fabric. The results are shown in figure 2.

Results

The models can fit the WAIS divide thin-section fabric samples well. The transition from girdle to single maxima deeper in the core due to increased horizontal shear is captured resonably well. Without stochastically variable stress grains, the model overpredicts the single maximum near the bottom of the core. In line with the results of Thorsteinsson (2002) for GRIP thin sections, we find that including nearest-neighbor interaction is important to enchance strain on hard grains. For these comparisons, accumulation is assumed to be constant, as is ice core temperature. More accurate data over time would likely improve the fit somewhat.

To understand the stochasticity which we may expect, we also repeatedly resampled the c-axis angles of the top thin section at 140m, with replacement, and forced the model with the WAIS divide data with the resampled (bootstrapped) samples as initial conditions. The bootstrapped sample c-axis angles have the same distribution as the original. With 400 grains, the resampled fabrics differ by a fair amount. Variability in EMD between samples stays at roughly the same magnitude throughout the model run. The results (fig 4) show that difference between the 5% and 95% quantiles of girdle EMD of the ensemble stays relatively consistent over time. Thus, initial perturbations of the fabric do not disappear over time. However, the EMDs of the resampled fabrics oscillate over time. The higher frequencey oscillations, to a large extent, do not covary between resampled fabrics. A fabric which was previously stronger than another may later become weaker, and vice-versa.

Fig. 2. Schmidt plot of fabrics produced under different flow scenarios. (a) Simple shear without recrystallization. (b) Uniaxial extension without recrystallization. (c) Simple shear with recrystallization. (d) Combined simple shear and uniaxial extension.
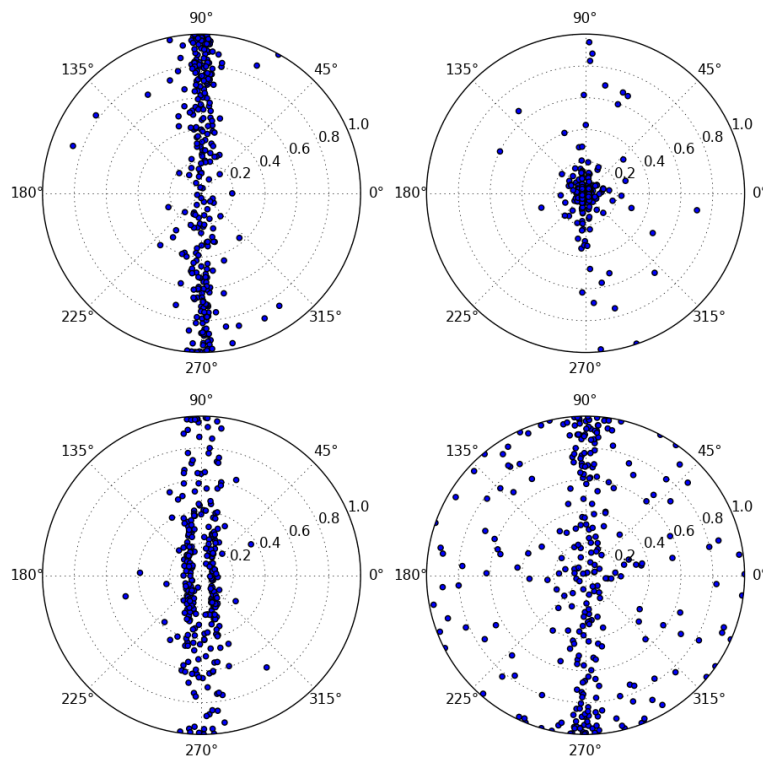
This is due to both the stochastic of recrystallization, and that nearest neighbors are chosen randomly. Similar behavior can be expected in ice sheets, as the number of nearest neighbors of each grain, and the sizes of the neighbors, can differ greatly from grain to grain. Now, these are limited samples of several hundred grains. Very large fabric samples evolve much more

Fig. 3. 90% confidence interval and median of evolution of the distribution of the fabric sample at the top of the core, inferred from repeated bootstrap samples of the thin section data. Two sample realizations are also included.
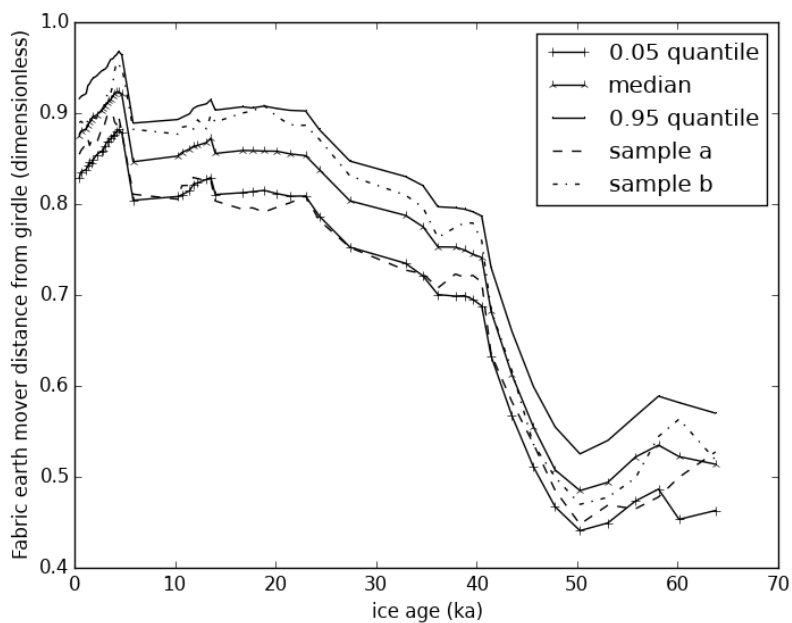
deterministically, as the stochasticity inherent in recrystallization and nearest neighbor selection does not affect bulk properties as much. However, these results do point to significant fabric variability on the meter-scale. This may be important in the development of small-scale flow features like boudinage. In addition, it is possible that the rapidly varying oscillations could cause transient flow on the meter-scale.

CONCLUSIONS

We showed a fabric evolution model which includes recrystallization and grain rotation. Grain growth and recrystallization depends on nearest-neighbor interactions. The model fits the WAIS ice core fabric data well. The models display a great deal of variability over time, with fabrics oscillating unpredictably over time. This suggests that random fabric variability may be important with small-scale flow. These results show that Jeffery's equation does a reasonably good job of predicting fabric orientation, despite the homogeneous strain assumption. Thus, the orientation-tensor-closure form Jeffery's equation is an appropriate simple model for grain rotation in large-scale flow models (as in Gillet-Chaulet and others (2006)). However, the efficient inclusion of recrystallization and polygonization into flow models is difficult. However, more parameterized treatments may be possible. Folgar and Tucker (1984) developed a version of Jeffery's equation for dilute fiber suspension orientations with rotary diffusion. Such an approach may provide a way forward to treat recrystallization.

Recent results (Montgomery-Smith, 2011) show that coupled Stokes-Jefferys equations modeling fiber suspensions can induce initial perturbations in the orientation distribution function to grow significantly in short amounts of time. The case of ice fabric is extremely similar. This opens up the possibility that small perturbations of the intitial fabric could grow into persistent large perturbations. This could be a source of the sometimes chaotic flow disturbances observed in some ice cores. Future work will include coupling of the fabric model to a fully anisotropic ice flow model to examine small-scale features such as boudinage and folding.

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ALGORITHM FOR THE FABRIC MODEL

Require: Fabric c-axis orientations $\mathbf{c_i}$, grain radii r_i, bulk strain rate D, vorticity tensor W, connectivity information C_{ij};

For each grain $\mathbf{g_i}$:

-Find local stress on each grain;

   -Find areas of each boundary between grains;

For each boundary of grain $\mathbf{g_i}$

   -Find grain growth rate over each boundary due grain boundary energy, dislocation density, and impurity content;

End For

   -Add contributions to grain growth of the boundary with each neighbor. Integrate grain growth over each boundary over the timestep;

   -Polygonize grain with probability p, depending on strain;

   -Rotate grain by integrating Jeffery's equation through the timestep;

End For

-Advance time by δt

-Return to **Start**.