A Parallel Simulation of a Quantitative Large-Strain Polycrystal Deformation

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1 Introduction

Predicting behaviour of materials when submitted to large strain is a fundamental problem of mechanics. In general, numerical simulation is one of the more widely used prediction methods. The problem related to numerical predictions is twofold. First, we have to define a simple reliable model which describes the major aspects of the evolution of material. Secondly, we have to face the need for computational power which conventional computers do not provide.

This paper deals with the problem of predicting the behaviour of polycrystals submitted to large strain. When polycrystalline metals are submitted to large strains associated with metal forming processes, such as rolling, extrusion, and forging, significant strain inhomogeneities occur at a grain scale. This is, first, due to the various crystallographic orientations of the grains, which induce a scatter of the flow stresses. However, two other factors can significantly affect the local behaviour of the aggregate: the aspect ratio of the grains (morphological texture) and the local distribution of the grains (topological texture). Such effects are not properly taken into account by the classical laws of mixture. In the present work, a new method was used to model the deformation of a polycrystal. It has been described elsewhere [4] and will be summarized in the next section.

To meet the computational requirements this model is simulated on a distributed memory parallel computer.

2 Outline of the model

The aggregate is represented by a two dimensional wraparound array of grains (see figure 1) generated in a plane (x_1, x_2) by a Voronoï tessellation [3].

The material is assumed to be incompressible and power law viscoplastic, i.e. $\sigma_i = k_i \dot{\varepsilon}_i^m$ where σ_i and $\dot{\varepsilon}_i$ are the flow stress and strain rate of grain i, respectively, k_i denotes the viscosity, and the strain rate sensitivity parameter $m = 0.2$ for all grains. The neighbourhood of each grain consists of the set of the n adjacent crystals (here, $n \approx 6$); it remains constant during straining.

The aggregate is submitted to plane strain compression along axis x_2, and elongates along x_1. For each overall strain step, all grains are considered in turn. The average viscosity of the neighbourhood of grain i is first calculated as:

$\overline{k_i} = \sum_{j=1}^{n} \alpha_i k_i$. The weighting coefficient α_i is proportional to the length of the boundary between grains i and j, and $\sum_{j=1}^{n} \alpha_j = 1$.

The strain rate of grain i is then derived as follows (it should be noted that the strain rate tensor reduces in the present case to a single component). The localization factor δ_i is : $\delta_i = \frac{(1+aF)(1-\tanh((b+cF)(\Sigma_i-1)))}{1+aF+(-1+dF)\tanh((b+eF)(\Sigma_i-1))}$. In this equation $F = \frac{2*\lambda_i}{\lambda_i^2+1}$, where λ_i is the aspect ratio of the grain, which is defined here as the ratio of the average intercepts of the grain parallel to the x_2 and x_1 axes. Σ_i denotes the hardness ratio $\frac{k_i}{\overline{k_i}}$, and a, b, c, d, and e are constants which have been determined numerically. The strain rate can then be written in the form: $\dot{\varepsilon}_i = \frac{\delta_i}{<\delta_i>}\dot{\varepsilon}_\infty$ where $\dot{\varepsilon}_\infty$ is the remote prescribed strain rate, and the average $<\delta_i>$ is extended over all the grains of the aggregate (each δ_i is weighted by the surface of the associated grain). The strain increment of each grain is then obtained as $d\varepsilon_i = \dot{\varepsilon}_i\, dt$. Finally, the overall viscosity of the polycrystal is : $k = \frac{<k_i\delta_i^m>}{<\delta_i>^m}$. In this work, each k_i was assumed to be strain dependent according to the classical equation: $k_i = \left[k_{si}^2 - (k_{si}^2 - k_{0i})\exp(-r_i\varepsilon_i)\right]^{1/2}$ where k_{0i} and k_{si} are the viscosity values for incipient straining (elastic limit), and at large strains (steady state), respectively, and r_i is a dynamic recovery parameter.

3 Parallel simulation

In the previous section we presented the model of a polycrystal deformation. Now we deal with the parallelism of the model and the problems which arise when implementing it on a real parallel computer.

It is obvious that the model is inherently parallel and has a synchronous behavior; therefore it is well suited to be implemented on a parallel computer.

However, it presents some pitfalls. This problem is similar to the graph partioning problem [2]. Indeed, the polycrystal aggregate can be viewed as a graph, the nodes corresponding to the grains and the edges corresponding to common edges of the grains. Optimal partioning algorithms are known to be very expensive; thus in this project, because our final goal is the simulation of continuous dynamic recrystallization, we decided a balanced partioning that fairly allocates the grains in the order their generation according to the Voronoï tessellation.

On the other hand, the computation of global variables requires gathering information disseminated throughout the network. In this work these global variables are calculated according to a master/slave approach. Each slave processor computes the partial values of these variables on the basis of the grains it owns, then sends the result to the master processor.

Now let us examine the processing of a grain. It consists in the computation of : k_i, $\overline{k_i}$, Σ_i, δ_i, $< \delta_i >$, $\dot{\varepsilon}_i$, the temporary coordinates of each vertex V_i^l, the final coordinates of all vertices, k and other global metrics of the aggregate. By gathering the information disseminated in the network, as described above, we obtain the following algorithms for each grain i and for the overall aggregate :

Deform_grain(i)
begin
compute k_i
get neighbours' information k_j
compute $\overline{k_i}$, Σ_i, δ_i
get global information $< \delta_i >$
compute $\dot{\varepsilon}_i$, σ_i and the temporary coordinates of each vertex W_i^l
get the neighbours' coordinates of the common vertices W_j^m
compute by the barycenter method the final coordinates V_i^l of all vertices
provide k_i, δ_i for the computation of k
end

Deform_aggregate
begin
for all i in parallel do
Deform_grain(i)
end

4 Implementation and results

We implemented the simulation of our model on a T805^{TM} transputer-based parallel machine. It consists of 16 transputers interconnected in a hypercube of dimension 4 (4×4 torus). This implementation uses the package D4414A of SGS - Thomson Microelectronics ANSI C Toolset [1] which incorporates a routing kernel. The performance of the simulation depends critically on the performance of this routing kernel.

The simulation algorithm described in section 3 could be implemented as described. All the grains located on the same processor are simulated as a single sequential process. In this case it is common that, when computing the status of some grains, the status of its neighbours is not yet available. This situation occurs when a grain has a neighbour located on a distant processor. Symmetrically, the neighbour has also the same view. Thus each pair of such grains must exchange their status. In order to avoid several exchanges of small messages, each processor sends one message to each of the other processors which hold neighbors of its grains; each message contains the status of the grains on the originating processor which have neighbours located on the destination processor. The overall algorithm thus consists of as many processes as processors, completely connected and exchanging through a small number of virtual channels at most two messages : the first for the values of viscosities and the second for the values of the temporary coordinates.

The initial mechanical characteristics of each grain are set randomly according to a uniform law (see figure 1). The overall rate strain $\dot{\varepsilon}$ is constant while the local one $\dot{\varepsilon}_i$ varies with the viscosity, the aspect ratio and the neighbourhood of the grain. Figure 2 shows the final aggregate after 1000 deformation steps with $\dot{\varepsilon} = 10^{-3}$ on the aggregate in figure 1.

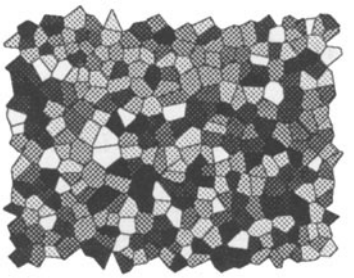

Fig. 1. An initial aggregate with 311 grains; the grey-level indicates the magnitude of viscosity

Fig. 2. The same aggregate after 1000 deformation steps, with $\dot{\varepsilon} = 0.001$; the grey-level indicates the magnitude of grain strain

Size of aggregate	60	311	2134	3847
Sequential time	0.143	0.743	5.100	12.242
Parallel time	0.0375	0.083	0.448	1.017
Speedup	3.82	8.89	11.36	12.04

Fig. 3. Time execution (in seconds) and speedup for a single step deformation

This simulation has permitted firstly to validate on larger-size aggregates of grains the material behaviour model described in section 2. Secondly, it allows us to obtain some new results about mechanical properties : only a very slight variation of the overall surface, has been obtained (0.02 %) and the three Hill macrohomogeneity conditions are fulfilled.

We can observe on figure 3 that the implementation strategy chosen is reasonably efficient. The speedup increases with the size of the aggregate.

5 Future work

This paper reported a parallel simulation of large-strain polycrystal deformation. A new model of deformation taking into account a large spectrum of deformation aspects (geometrical, topological and mechanical) was developed and validated.

The model is presently being extended to take into account the occurrence of continuous dynamic recrystallization at large strains. For that purpose, when a given grain i has reached some prescribed level of stored energy $w_i = \int k_i \dot{\varepsilon}_i^m \, \mathrm{d}\varepsilon_i$, it is divided into new grains by a Voronoï tessellation, in the same manner as for the original structure.

The parallel simulation of continuous dynamic recrystallization requires dynamic load balancing. The related study is in progress.

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