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A Time Split Strategy for Coupling Mechanical Stress Fields with Grain Scale Phenomena using MPM

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ABSTRACT

There are many applications where the behaviour at the microstructure scale is directly coupled with macro or continuum scale fields. For example, the grain restructuring and transport of micro- and nano-scale bubbles in nuclear reactor fuel is directly coupled with the combined continuum mechanical stresses and thermal gradient. Monte-Carlo methods can simulate microstructural evolution such as grain growth and bubble migration; however, these are not directly coupled with the mechanical and thermal stresses. The evolution in microstructure and mechanical phenomena such as cracking, creep, and swelling are intimately related and must be directly coupled in high fidelity simulations which are now enabled by modern multi-processor computer clusters.

We will present a time-split method which directly couples grain boundary motion and bubble transport at the microscale with the continuum mechanical stresses and thermal gradient. The basis for this method is the Material Point Method (MPM)[1]. The domain is represented by computational particles which contain the solution of the continuum mechanics equations which includes its stress tensor; each material point represents a particular material type or polycrystal grain orientation. Our current problems of interest are generally quasi-static; a lagrangian background mesh is used to minimize the cell crossing issues exhibited by eulerian grid based MPM methods. Independent of the MPM algorithm, all of the computation particles are also operated on by a Monte-Carlo Potts Model which statistically determines a system response based on the minimization of the local Gibbs free energy. We use a Potts-Glauber model for the grain boundary restructuring and a Potts-Kawasacki model for the bubble transport; these are combined in a statistical time sampling strategy as a kinetic Monte-Carlo (kMC) model. It is critical that the Monte-Carlo transport algorithms be calibrated to include a time scale for coupled applications.

The microstructure phenomena are weakly coupled in time with the stress and thermal fields for our applications. That is the microstructure time constant is much longer than the characteristic mechanical stress time constant (i.e. the material wave speed). Therefore, we solve these in a decoupled manner: the MPM algorithm is performed on a fixed microstructure and then the resultant mechanical and thermal stresses are used in the kMC model to advance the microscale.

Figure 1 illustrates the Potts-Kawasacki algorithm. The 2D domain is composed of four different grains with periodic boundary conditions on the domain; all materials are represented as MPM material particles. Initially gas bubbles are randomly inserted into the material; this is illustrated by the left figure with the dark areas representing the gas bubbles. The system, without thermal or mechanical stresses, will evolve to a state where the bubbles are clustered at grain boundaries as shown in the figure on the right.

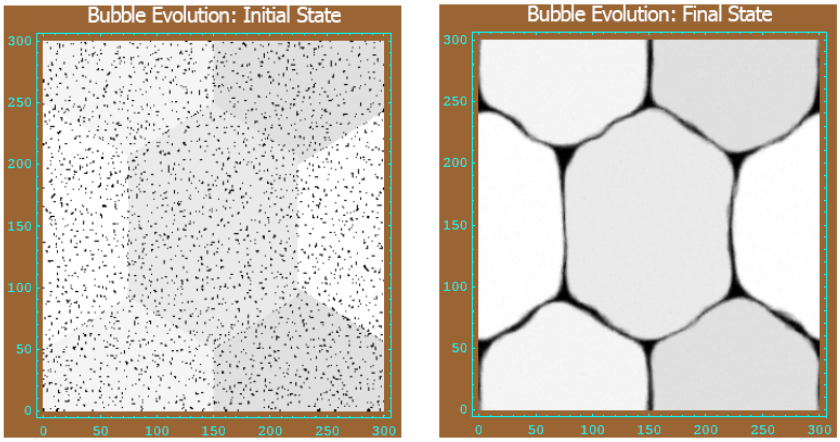
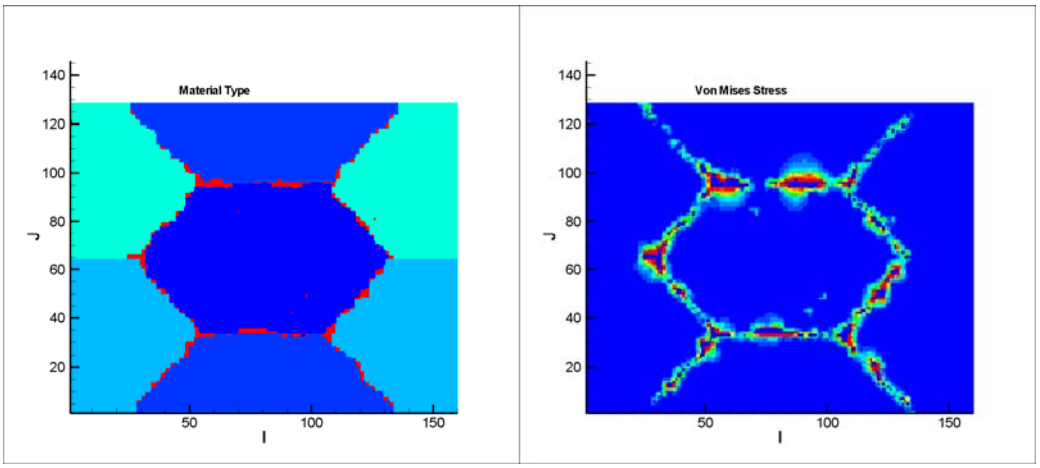


Figure 2 illustrates the stress coupling between bubbles and solid material. For this simulation, the material composition is fixed as shown in the left figure; the red regions represent gas material points. The gas pressure, a scalar field, is set to a fraction of the material yield stress. The domain boundaries are allowed to move and the material will swell. Contours of the von Mises stress at a early time are shown in the right figure; the local stress concentration in the solid material is clearly illustrated.



Coupled simulations with grain restructuring and bubble transport in stress and temperature fields will be presented.

REFERENCES

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