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NSR&D FY17 Report: CartaBlanca Capability Enhancements

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Summary

Over the last several years, particle technology in the CartaBlanca code has been matured and has been successfully applied to a wide variety of physical problems. It has been shown that the particle methods, especially Los Alamos's dual domain material point method, is capable of computing many problems involves complex physics, chemistries accompanied by large material deformations, where the traditional finite element or Eulerian method encounter significant difficulties. In FY17, the CartaBlanca code has been enhanced with physical models and numerical algorithms. We started out to compute penetration and HE safety problems. Most of the year we focused on the TEPLA model improvement testing against the sweeping wave experiment by Gray et al. [1], because it was found that pore growth and material failure are essentially important for our tasks and needed to be understood for modeling the penetration and the can experiments efficiently.

We extended the TEPLA mode from the point view of ensemble phase average to include the effects of finite deformation. It is shown that the assumed pore growth model in TEPLA is actually an exact result from the theory. Along this line, we then generalized the model to include finite deformations to consider nonlinear dynamics of large deformation. The interaction

between the HE product gas and the solid metal is based on the multi-velocity formation [2]. Our preliminary numerical results suggest good agreement between the experiment and the numerical results, pending further verification.

To improve the parallel processing capabilities of the CartaBlanca code, we are actively working with the Next Generation Code (NGC) project to rewrite selected packages using C++. This work is expected to continue in the following years. This effort also makes the particle technology developed with CartaBlanca project available to other part of the laboratory. Working with the NGC project and rewriting some parts of the code also given us an opportunity to improve our numerical implementations of the method and to take advantage of recently advances in the numerical methods, such as multiscale algorithms.

1 Ensemble Phase Averaged Equations

Ensemble averaging method has been used in statistical mechanics to study motion of molecules and to obtain macroscopic governing equations and their closures. Batchelor [3] first used it to study effective viscosity of particle suspensions. Ensemble phase average is a phase specific averaging method and has been used to derive average equations for multiphase flows [4, 5]. Lately [2], the ensemble phase average method has been applied to multi-material interaction problems. In the present work, we use the method to study the tensile plasticity (TEPLA) model [6, 7, 8], which considers effects of void growth in plastic metal deformation. In principle, one can use the equations in [2] directly to write the average equations for both the solid and the voids and study their closures. This approach is used in the derivation of the basic equations for bubbly flows [9]. However, unlike bubbles in a liquid, for voids in a solid, the relative velocity between void and the solid is negligible. For this reason, we only need to study average motion of the solid, without explicitly solving for velocity field for the voids to avoid the complexity of two velocity fields. The effect of the voids is represented in the closure relations for the bulk material.

In multiphase flows, the voids are often regarded as bubbles filled with a gas phase that can response to volume change by pressure. The pressure inside the voids is comparable to the surround fluids. In cases of metal, which we can also regard the voids are filled by air, but its pressure response is so weak compared to metal stress. The pressure inside the void is negligible. It is this difference that results in the different forms of the momentum equations. If the voids

are replaced by some other material with significant inertia, a full multiphase treatment for the void is needed together with interaction forces and stresses between the materials.

The original tension plasticity (TEPLA) model is for small deformation and small porosity. In this work we, extend it to finite porosity and finite deformations. The original TEPLA equation for porosity growth and material density evolution are still correct for problems with finite deformation and finite porosity. The same as in the original TEPLA model, we assume that the pressure obeys the Mie-Gr niesen equation of state. The only extension needed here is the stress calculation in cases of finite deformation.

We assume deviatoric stress is hyperelastic. We use the velocity gradient to evolve the deformation gradient and the elastic deformation gradient and then use the elastic deformation gradient to calculate the deviatoric part of the Cauchy stress, while the pressure component of the stress is calculated from the Mie-Gr niesen equation of state.

To consider plasticity, we use the Gurson surface which is a function of the deviatoric stress, pressure, and porosity in the metal. Within the surface, the metal deforms elastically. The stress is not allowed to be beyond the surface. If a stress state moves beyond the surface, plastic deformation occurs to correct the stress back on the surface using the normal return rule. According to the rule, the material deforms plastically in such a way that plastic strain is normal to the Gurson surface.

2 Numerical schemes

For materials undergoing large deformations, typical numerical methods encounter two difficulties. The first one is about the numerical discretization of the material to ensure that the gradients are calculated correctly and the conservation laws are accurately enforced. The second difficulty is about the nonlinear material behavior. These two difficulties are often referred as geometric and physical nonlinearities. With the particle technology, the geometric nonlinearity can be handled easily, allowing us to focus more on the physical nonlinearity. The ability of the particle technology to track history of material, make us possible to calculate the deformation gradients accurately. We find that the typical linear update of the quantity could lead to significant errors as shown in Fig. 1. The figure shows the error of the deformation gradient of a rigid body rotation. In a rigid body rotation, the deformation gradient is an orthogonal tensor. The typical

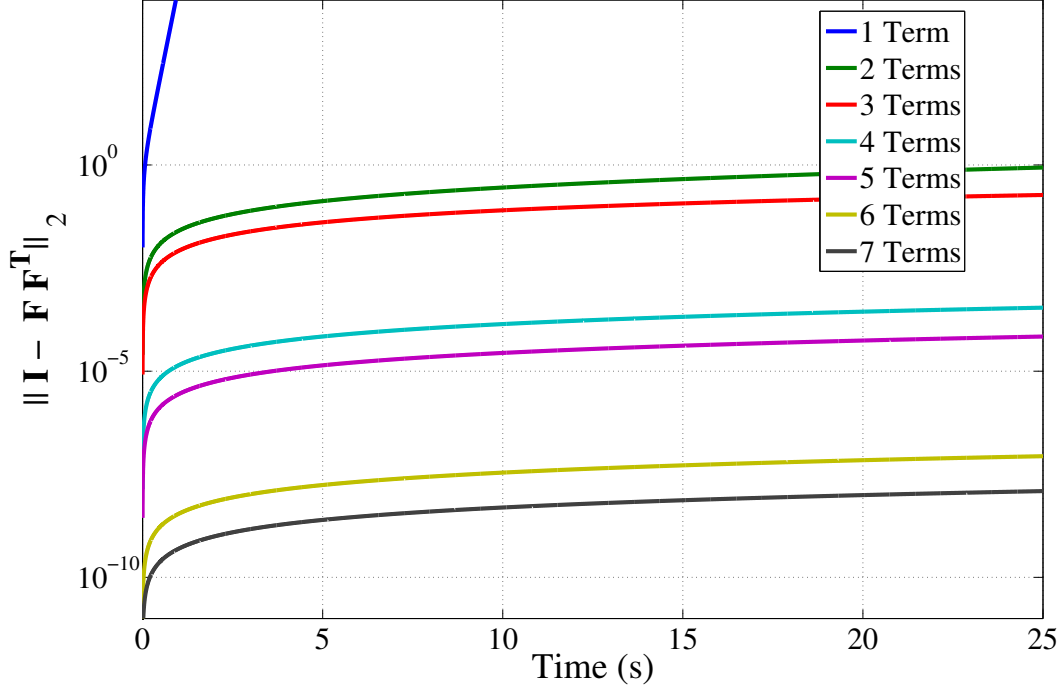


Figure 1: The divergence from orthogonality of the computed deformation tensor, $\mathbf{F}$, is plotted versus time during a test rotation for n terms used in the Taylor expansion of the tensor exponentiation.

linear update corresponds to the blue curve on the top of the figure showing significant error for a case with rotational angular velocity 100 rad/s.

The figure shows different number of terms used in the Taylor expansion to compute the deformation gradient. The error decreases with the increasing number of terms used as expected. Interestingly, the accuracy improvement does not happen uniformly, as can be seen in the figure. The error drops significantly going from an odd-number of terms to the next even number of terms, and does not change significantly by increasing the number of terms used from an even number to an odd number. Thus, we conclude that the Taylor series should be truncated no sooner than the quadratic term, and additional terms should be added in pairs. In CartaBlanca, the default is now set to 4 terms with a numerical scheme to accelerate the convergence.

To ensure numerical stability, the tension plasticity model is solved implicitly. The basic solution strategy has been published [10] and reported last year. In the current FY, we extended

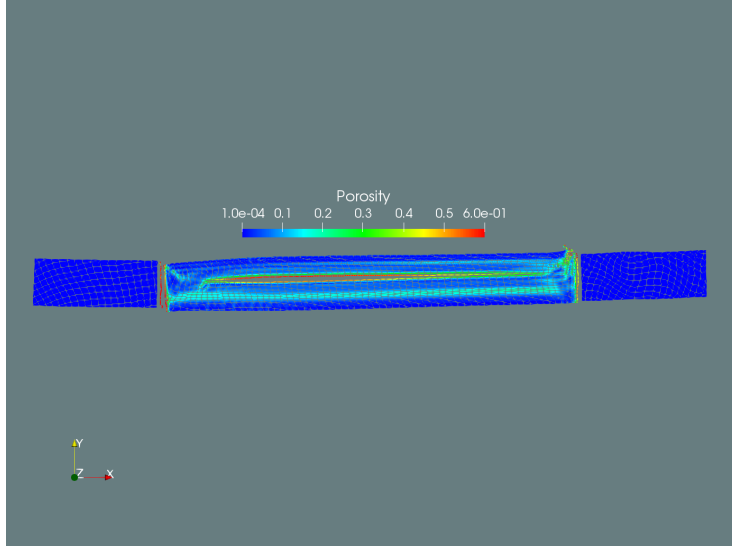


Figure 2: CartaBlanca result of the porosity after passage of a sweeping oblique shock.

the method and made it applicable to finite deformations. More importantly, we significantly improved the robustness of the solution method.

The new improvement is based on the mathematical discovery of a property relating the normal return rule of the plasticity theory to the trajectory on the pressure–deviatoric stress (P, τ) plane. Since the stress state is in a 6-dimensional space, (3-dimensional for a two-dimensional problems), by mapping the stress state to the two-dimensional (P, τ) plane, we reduce the difficulty of the solving the equations. Currently, we are working on a publication describing this improved numerical scheme in detail.

With this extended TEPLA model and the new numerical scheme, we use CartaBlanca to simulate the sweeping wave experiment [1]. The preliminary results are shown in figures 2 and 3. The numerical results depend slightly on the measuring positions and material parameters, such as the porosity at failure. For further comparison, we plan to work with the experimentalist to figure out the details in the next few weeks.

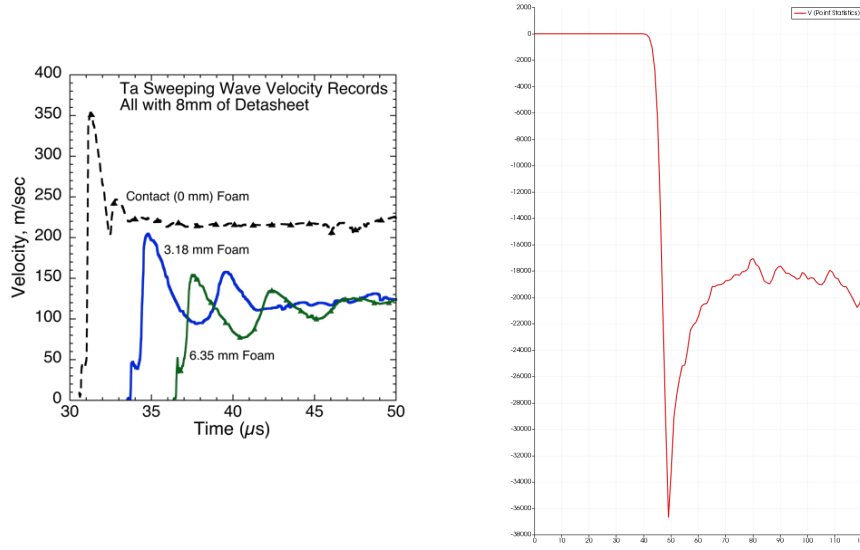


Figure 3: Preliminary comparison of velocity. The y axis is reversed in these figures. The x (time) axes are not properly scaled (should be by a factor 4) and aligned yet.

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