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Interface reconstruction in two- and three-dimensional arbitrary Lagrangian-Eulerian adaptive mesh refinement simulations

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Abstract.

Modeling of high power laser and ignition facilities requires new techniques because of the higher energies and higher operational costs. We report on the development and application of a new interface reconstruction algorithm for chamber modeling code that combines ALE (Arbitrary Lagrangian Eulerian) techniques with AMR (Adaptive Mesh Refinement). The code is used for the simulation of complex target elements in the National Ignition Facility (NIF) and other similar facilities. The interface reconstruction scheme is required to adequately describe the debris/shrapnel (including fragments or droplets) resulting from energized materials that could affect optics or diagnostic sensors. Traditional ICF modeling codes that choose to implement ALE + AMR techniques will also benefit from this new scheme. The ALE formulation requires material interfaces (including those of generated particles or droplets) to be tracked. We present the interface reconstruction scheme developed for NIF's ALE-AMR and discuss how it is affected by adaptive mesh refinement and the ALE mesh. Results of the code are shown for NIF and OMEGA target configurations.

1. Introduction

Understanding debris and shrapnel production is very important in high power laser facilities such as NIF, LMJ and Omega, because the energetic droplets and fragments have the potential to damage optics and diagnostic devices. Models that predict the formation, size and trajectory of fragments and droplets can be used to develop designs that minimize the formation or potential effects of damaging shrapnel [1]. Modeling such systems requires significant volumes of empty space in which to track problem geometry and formation of debris/shrapnel. NIF's ALE-AMR code addresses many of these challenges by combining a deformable (ALE) mesh with structured adaptive mesh refinement. An ALE formulation responds to material movement and provides some self-adaptation while postponing or avoiding mesh entanglement. AMR refines the mesh as needed, allowing large empty regions to be efficiently modeled without sacrificing accuracy. The interface reconstruction scheme we describe in this paper is required to model the sub-zonal physics necessary for describing the trajectories and physics of particles created when a target dismantles.

2. Interface Reconstruction in NIF ALE-AMR

NIF's ALE-AMR incorporates an arbitrary Lagrangian-Eulerian (ALE) staggered mesh simulation algorithm with a locally structured adaptive mesh refinement (AMR) framework, based on the work

of Anderson, et al. [2, 3]. An ALE algorithm allows the simulation mesh to either follow the material (Lagrangian), be fixed (Eulerian) or utilize an arbitrary mesh that is somewhere in between (ALE). As such, an ALE simulation can postpone mesh entanglement that may limit purely Lagrangian simulations by relaxing the mesh movement. Furthermore, this also provides a certain amount of natural self-adaptation as the grid follows the flow dynamics. The basic algorithm consists of Lagrange plus Remap (ALE) followed by regridding/rezoning (AMR) [2]. One consequence of an ALE (or Eulerian) algorithm is that material interfaces, which are tracked naturally by a conformal Lagrangian mesh, must be tracked in some other manner. The most prevalent methods for interface reconstruction involve storing volume fractions of the material components within mixed zones and reconstructing interfaces as needed [4, 5, 6, 7]. The following sections present how interface reconstruction has been implemented in the NIF-ALE-AMR algorithm.

2.1. Lagrange Step

During the Lagrange step, the forces acting on the nodes (due to zonal pressure, stress components and imposed loads) and the resulting nodal accelerations and displacements are evaluated. Within mixed zones the pressures and stresses are weighted by the volume fractions of the component materials to obtain composite quantities [6, 8]. Mesh deformations are used to determine volumetric and deviatoric strain rates, which must be partitioned amongst component materials in mixed zones, often altering the volume fractions. In NIF's ALE-AMR strains rates are partitioned based on the material volume fractions and the bulk moduli for volumetric component or the shear moduli for deviatoric components. The strain rates and the current stress and material state (plastic strain, damage, etc.) for each material (in clean or mixed zones) are then used to update the internal energy ($p\,dv$ work) and the stress state—including hardening and failure—based on appropriate material models, e.g., the Johnson-Cook model [9]. If failure is detected a special *void* material may be inserted. In subsequent steps this may grow and coalesce with void in other zones—providing a mechanism for fracture and debris formation (for additional details see Ref. [10]. The effect of void insertion is demonstrated in the simulation results.

2.2. Remap

The remapping or interpolation of the nodal and zonal quantities to a new mesh configuration (ALE or Eulerian) is treated as an advection problem, first determining the material volumes to be advected between zones during the remap step. Once this is determined, the zonal and nodal quantities are advected along with the volume. In mixed zones, the contribution, if any, of the component materials to the advected material must be determined. We utilize a standard method that treats the volume fractions of neighboring zones to approximate the orientation of the material interfaces within a donor zone and then to select a likely ordering for the materials to be advected [11]. This avoids explicitly reconstructing the interfaces during the advection step and has been shown to work well in practice. In clean zones the gradient of the advected quantities may be used to obtain a second-order accurate scheme. Such a gradient cannot, in general, be constructed for the components of mixed zones and necessitating a first-order constant-valued scheme for the advection of mixed quantities.

2.3. Adaptive Mesh Refinement

User defined criteria are used to identify regions that may be coarsened or refined—refining the mesh to maintain accuracy in regions with rapidly changing dynamics and coarsening in less dynamic regions to reduce computational expense.

In the case of clean zones, the coarsened quantities are averaged by volume or mass weighting. The same method may be used for mixed zones, with the volume fraction of the coarsened zones $V_{f,c}$ being the volume weighted average of the volume fractions of the fine zones being coarsened. Zonal quantities are coarsened in a similar manner: weighted by volume fractions for density, pressure and deviatoric stresses, etc. and by mass fractions for internal energy. Nodal velocities are determined in the same way for mixed and clean zones, albeit using the composite masses from mixed zones.

Refinement poses a much more difficult problem. In a clean coarse zone, the zonal and nodal quantities may be interpolated to the new refined zones by defining a gradient in terms of the neighboring zones. As mentioned in the previous section, we cannot utilize gradient based interpolation for mixed zones. Furthermore, we must first determine the composition of the refined zones (clean or mixed and volume fractions). This requires an explicit reconstruction of the interface. From the stored volume fractions we again calculate the orientation of each interface and then solve for the location that results in the appropriate truncated volume within the coarse zone. Intersecting this reconstructed interface with the refined zones yields the necessary compositions and associated volume fractions.

In 1D, evaluating the truncated volume (length) is trivial. In 2D, the regions formed by truncating a general quadrilateral with linear interfaces will be polygonal—the volume (area) of which may be easily calculated. In 3D, the zones are general hexahedra, bounded on six sides by doubly ruled surfaces (see Figure 1). We have developed a method, similar to that proposed by Kothe, et al. [12], that may be used to determine the volume of a general (including degenerate) hexahedron truncated by a plane. Figure 1), diagrams how the method works for onion-skin topologies (multiple interfaces are non-intersecting within a given zone). A possible alternative breaks each zone into 27 tetrahedrons and then evaluates the plane-tetrahedron intersections [13]. Once the composition of the refined zones have been determined, the zonal quantities may be assigned using the constant values for the mixed quantities of the parent coarse zones. The nodal velocities again depend on the composite quantities and are interpolated in the same manner for clean and mixed zones.
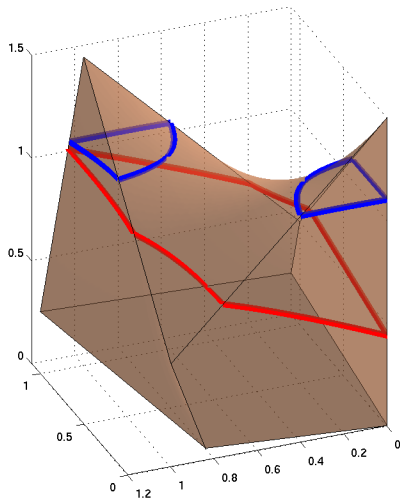

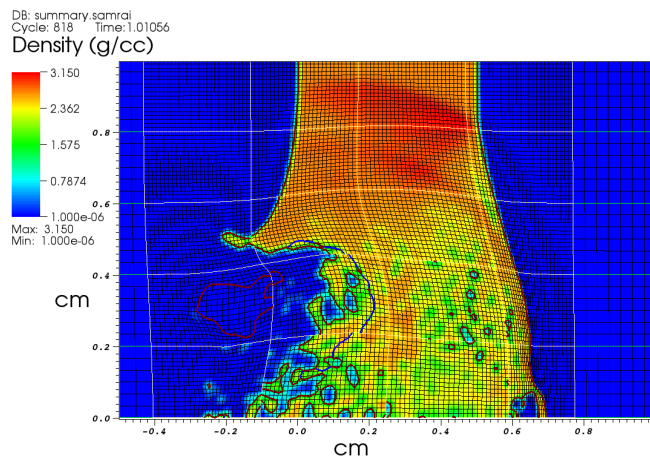**Figure 1.** Truncated arbitrary hexahedron for 3D interface reconstruction

Figure 2. Spall formation aluminum plate impacted by steel hohlraum

3. Simulation Results

We present two example simulations of interest to high energy laser systems: An aluminum plate impacted by a steel (hohlraum) projectile and a cooling ring. The plate in this simulation (see Figure 2) is 0.5 cm thick 6061-T6 Aluminum. A steel hohlraum impacts the plate with a velocity of 750 m/s. As the shock wave passes through the plate, the rarefaction wave returns from the back (right) side causing failure in the material. As failure is predicted, void is inserted into failed zones which leads to the formation of spall planes (visible on the right side of the plate).

The second simulation investigates the effect on fragment formation of thinning a copper cooling ring. Two rings were simulated with similar geometries (r_o = 5.207 mm, r_i = 0.8382 mm, t = 0.0508 mm), but the outer radius of one is reduced to 1.27 mm over three quarters of the ring. The inner surfaces of
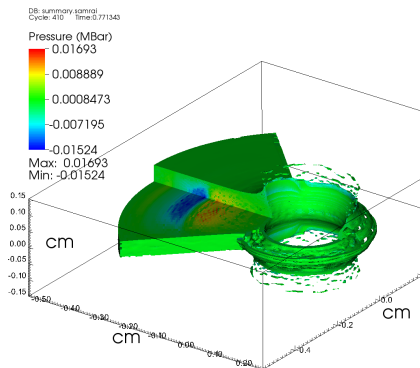
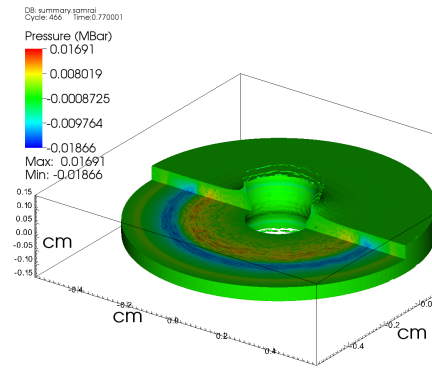**Figure 3.** Notched Cu cooling ring showing spall formation

Figure 4. Full Cu cooling ring showing little debris formation

the rings (to a depth of approximately 0.1 mm) were the loaded with an impulsive radial velocity of 2000 m/s. The results at approximately 0.7 µs are shown in Figures 3 and 4, where the debris formed near the lip of the inner radii are similar for both simulations, but a significant amount of spalling is predicted around the circumference of the reduced ring (Figure 3, which is undesirable. Contours are pressure, with compressive (red) and tensile (blue) waves evident in the cut-away.

4. Conclusions and Recommendations

NIF-ALE-AMR is a promising tool for predicting late-time dynamics and shrapnel and debris formation in high energy laser facilities. We have developed an interface reconstruction algorithm that is compatible with the arbitrary mesh geometries inherent in ALE simulations as well as the adaptive mesh refinement. Example simulations presented here illustrate the power of NIF-ALE-AMR as a predictive modeling tool.

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