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Ejecta source and transport modeling in the FLAG hydrocode

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A B S T R A C T

We present the ongoing development and implementation of an ejecta model in the FLAG hydrocode. Ejecta is the term given to particulate matter that is produced at the free surface of a material subject to extreme shock loading. Following shock propagation into a material and reflection at its free surface, conditions may be sufficient to induce phase changes, damage, or fragmentation at the surface. The dynamics of the fragmentation may be such that a ‘‘cloud’’ of particulate matter forms and propagates away from the material.

Modeling such phenomena in a continuum hydrodynamics code challenges the assumptions underlying the numerical approximations made in the hydrodynamics. The representative scales for the particulate matter are often much smaller than the representative scales for the bulk material producing the ejecta. However, this scale separation allows for statistical descriptions of ejecta that are compatible with continuum mechanics.

Earlier work documents an initial effort in modeling ejecta in the FLAG hydrocode. The FLAG hydrocode computes continuum mechanics solutions for fluid and solid materials in an Arbitrary–Eulerian–Lagrangian (ALE) framework. To model ejecta in FLAG, a hybrid particle-continuum representation was defined that allows for coupling with continuum materials on large (bulk) scales. Numerical models were developed and implemented for particle production (sourcing) as well as for solving the particle equations of motion. The numerics were shown to conserve mass, momentum and energy, and preliminary results were given for modeling drag and volume effects.

This work documents recent advances in source and transport models. Spatial and temporal dependencies have been added to the source models to account for geometric free-surface variations, mesh dependence, and shock loading. More physically relevant drag models have been implemented that include Reynolds number effects. These will be presented along with test results verifying the models. A FLAG model of an actual ejecta experiment will also be presented.

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1. Introduction

1.1. Experimental background

Subject to extreme shock loading, materials may undergo thermodynamic changes and phase changes as well as irreversible plastic deformation and damage. Following shock propagation through a material, conditions at the shock breakout with the material free surface may be sufficient to induce particle fragmentation. This fragmentation is known as ejecta [1,2] and is observed as streams or ‘‘clouds’’ of particulate matter that form and propagate away from the material. The nature and properties of ejecta source and transport have been the subject of ongoing research through experiment and analysis [3–5].

An example of an ejecta experiment is shown in Figs. 1 and 2. In this experiment, a small tin sample is loaded from one end by a high explosive charge. The high explosive is detonated, sending a detonation wave that propagates into the tin sample as a shock. The shock propagates through the sample and breaks out of the tin free surface, inducing ejecta generation. A series of photographic images is shown in Fig. 3 to illustrate this phenomenon. As shown in this figure, the ejecta cloud appears and propagates to the right. The statistical properties of the ejecta cloud contribute to the appearance of density variations in the figure.

The spatial and temporal scales present in ejecta pose a challenge to computational modeling. The damage processes during shock breakout that lead to ejecta generation occur over smaller scales compared to the bulk material motion. Particle sizes can be similar to or smaller than bulk material grain sizes, which are usually smaller than typical mesh resolution settings for continuum simulation. Furthermore, ejecta particle populations can be much larger than mesh cell counts for typical simulations.

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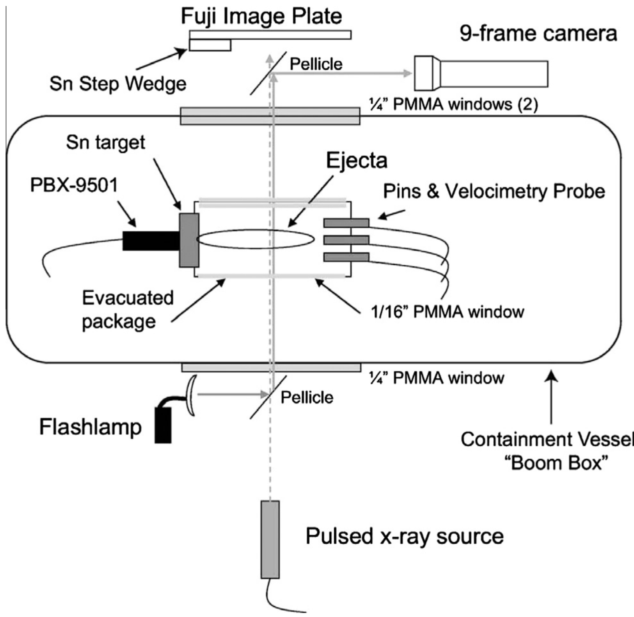

Fig. 1. Schematic of an ejecta experiment. From [4].

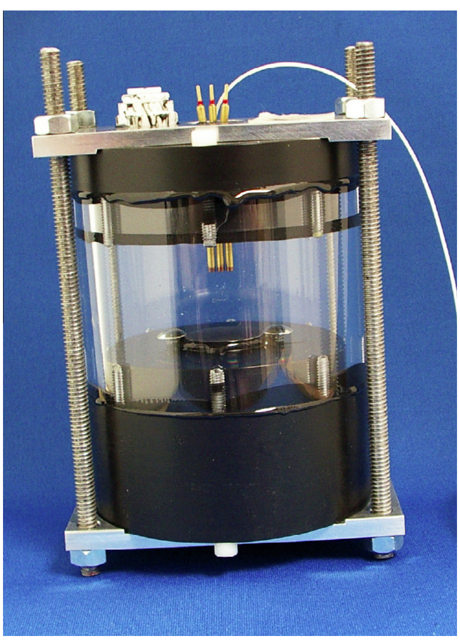

Fig. 2. Photo of an ejecta experiment. The high explosive and tin sample are oriented to produce ejecta directed upwards in this image. From [4].

1.2. Theoretical background

This work represents an ongoing effort to model ejecta phenomena using the FLAG hydrocode. FLAG is a continuum hydrodynamics research code developed at Los Alamos National Laboratory, with capabilities for modeling shock hydrodynamics experiments involving multiple materials at high strain rates [6,7]. The FLAG code has been used to model the continuum hydrodynamics of experiments such as those shown in Figs. 1 and 2. However, as discussed above, FLAG is not suited to model ejecta phenomena through brute-force numerical resolution of particles (as small-scale continua) and their source and transport. However, the separation of scales described above allows for a statistical description of ejecta that is compatible with continuum mechanics.

One fruitful approach for particle simulations is based on a distribution function $f(t, x, m_p, u_p, e_p, \ldots)$, which may be regarded as a phase space density of particles of mass m_p, velocity u_p, internal energy e_p and so forth. This type of analysis is naturally based on the Boltzmann equation or variants thereof (referred to as the Vlasov-Boltzmann, spray or Liouville equation in the references cited here). For instance, for particles of uniform mass m_p, a simple form is found in [8–10]:

$$\partial_t f + u_p \cdot \nabla_x f + \nabla_{u_p} \cdot (f\Gamma) + \partial_{e_p}(f\phi) = Q \quad (1)$$

in which Γ and ϕ are the rates at which momentum and internal energy are transferred to a given particle from the surrounding fluid, and Q is the collision kernel.

As an example, Monte-Carlo-type particle methods in the KIVA code [11] approximate f as a sum of Dirac delta functions. We may regard this as the foundation of the hybrid fluid-particle work described in this paper.

Earlier work by the authors has introduced a hybrid particle-continuum representation into FLAG for modeling ejecta [12]. That work included an initial implementation of numerical methods for the generation and transport of ejecta that are consistent with conservation and other properties of the continuum hydrodynamics discretization.

This work documents recent advances in source and transport models for the ejecta capability in FLAG. Spatial and temporal dependencies have been added to the source models, and more physically relevant drag models have been implemented. These will be discussed in the next section. Model validation with analytical test cases will be presented in Section 3. Finally, simulations of an actual ejecta experiment will be presented in Section 4.

2. FLAG MP-PIC methodology

This section describes the FLAG ejecta capability in the framework of particle-in-cell methods. The discrete equations of motion for the entire system is given. This section then presents new ejecta source and transport models that have been implemented into FLAG.

2.1. FLAG MP-PIC

The FLAG ejecta capability is formulated as a Multiphase Particle-in-Cell (MP-PIC) method, where the simulation capability includes distinct continuum and particle components. An example of a FLAG MP-PIC simulation is shown in Fig. 4, where numerical particles coexist with a continuum hydrodynamics mesh. Andrews and O'Rourke outlined the MP-PIC method in [13] in the context of modeling liquid sprays and gas–liquid mixtures under combustion. The components of the FLAG ejecta capability are listed below.

2.1.1. Continuum representation and dynamics

The FLAG hydrodynamics code is well suited to model the continuum aspects of ejecta experiments such as those shown in Figs. 1 and 2. FLAG modeling capabilities include solid and fluid continuum mechanics at high strain rates, shock physics, and material strength, plastic deformation, damage, and contact. The FLAG mesh representation is fully unstructured and may include split ends (dendrites) and arbitrary polygons (two-dimensions) and polyhedra (three-dimensions).

The underlying numerical hydrodynamics method follows from a staggered grid, compatible Lagrangian discretization formulated by Don Burton [6,7]. Having an Arbitrary-Lagrangian–Eulerian