New Capabilities for Modeling Creation and Breakup of Ejecta in the FLAG Code

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Abstract

We report new developments in the particle-in-cell ejecta package in the FLAG Lagrange/ALE continuum mechanics code. In particular, we have implemented a new ejecta source model based on the phenomenology of the Richtmyer-Meshkov instability, and the Taylor Analogy Breakup (TAB) model for the breakup of ejecta particles (droplets).

The Richtmyer-Meshkov source model is based on the hypothesis that mass ejection from shocked metal surfaces occurs principally when the surface is liquid upon shock release, and that therefore the ejecta are droplets necked off from the "spikes" in a Richmyer-Meshkov fluid instability. A theoretical model[1] for the bubble and spike growth rates is used to predict the mass ejection rate. Implementation details and sample calculations will be presented.

The Taylor Analogy Breakup (TAB) model was developed by O'Rourke and Amsden[2] to model the breakup of droplets in sprays in the KIVA code. It is based on a second-order ODE model of the variations in the equator of a droplet about its equilibrium position as a damped harmonic oscillator. Oscillations are driven by the motion of the drop relative to the background gas, with a restoring force due to surface tension, and damping due to the viscosity of the liquid. The numerical implementation in FLAG solves the ODE, testing at each cycle whether the distortion of each droplet has exceeded a threshold for breakup. When that condition is satisfied, a distribution of daughter droplet sizes and a typical lateral velocity spread are modeled, and the parent drop is replaced in the simulation by a daughter droplet sampled from the size distribution and the possible lateral acceleration directions.

The TAB model and its implementation in FLAG will be described, and sample verification and validation calculations will be presented.

[1]W. T. Buttler, D. M. Oró, D. L. Preston, K. O. Mikaelian, F. J. Cherne, R. S. Hixson, F. G. Mariam, C. Morris, J. B. Stone, G. Terrones, and D. Tupa, "Unstable Richtmyer-Meshkov Growth in Solid and Liquid Metals in Vacuum," *J. Fluid Mech.* **703**:60-84 (2012).

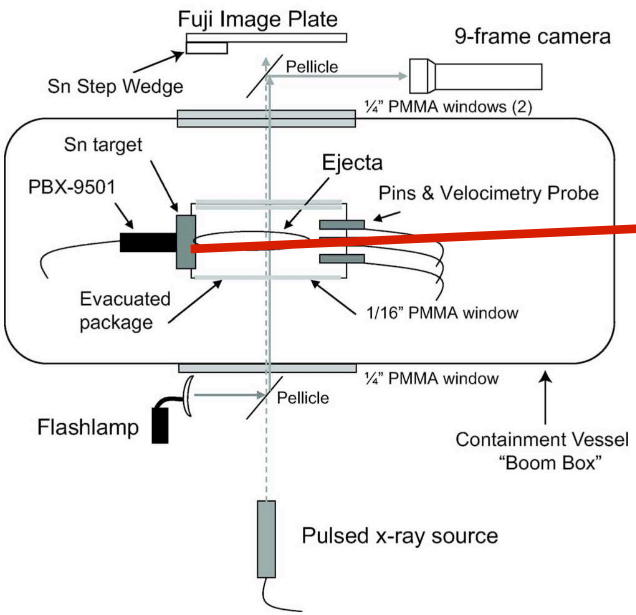
[2]P. J. O'Rourke and A. A. Amsden, "The TAB Model for Numerical Calculation of Spray Droplet Breakup," Los Alamos National Laboratory report no. LA-UR-87-2105 (revised), 1987.

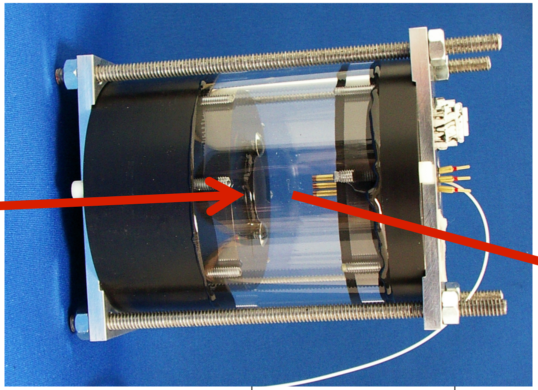
Outline

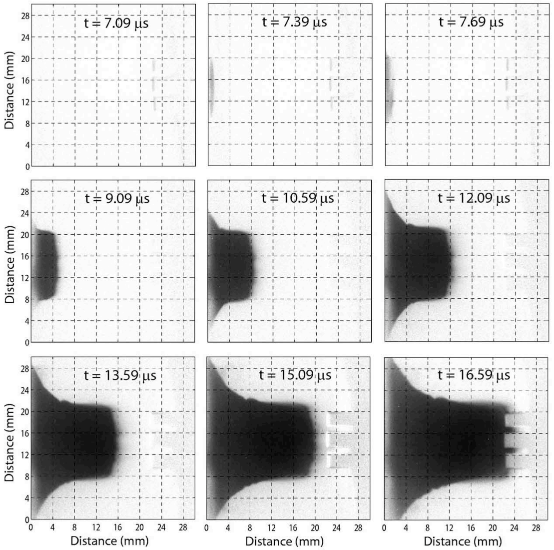
- Motivation and general features of ejecta package
- Richtmyer-Meshkov Instability (RMI) source model
- Taylor Analogy Breakup (TAB) model
- Plans for a unified model

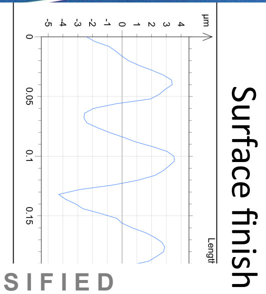
Motivation: Ejecta and modeling ejecta experiments

- Extreme shock loading may cause damage and failure at material free surfaces, producing particulate fragmentation known as ejecta.
- Theories, experiments, and modeling involve a wide range of solid and fluid mechanics at relevant spatial and temporal scales.





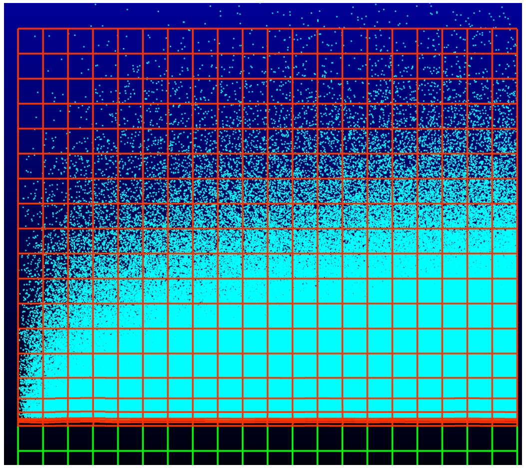




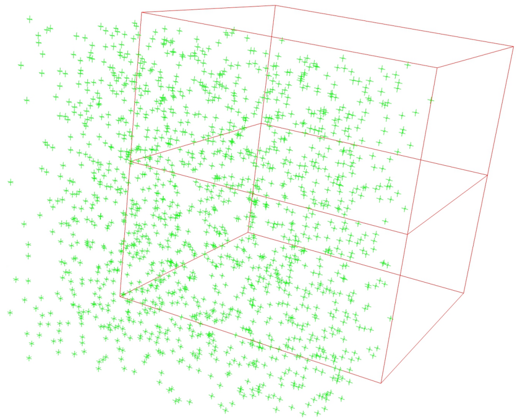
See many experimental papers by W. T. Buttler, R. T. Olson, M. B. Zellner and coworkers

An MP-PIC (Particle-Mesh) formulation is used to model ejecta in FLAG.

- (Super) particles represent packets of multiple physical particles.
  - Tracking individual physical particles is expensive, so allowing computational particles to represent many physical particles reduces cost. The tradeoff is the statistical resolution.
- While FLAG hydro advances the continuum equations of motion, a distinct solver is implemented to advance particle equations of motion.
  - Particle positions and velocities are maintained in 3D
  - Positions and velocities are projected/rotated into the space of the mesh (e.g., 2D axisymmetric)
  - Projected positions are located in cells of the hydrodynamics mesh
- Particle-fluid coupling (for e.g. drag forces) requires
  - Summing particle quantities (mass, volume) over zones
  - Interpolating continuum information from mesh zones and points to particles



Ejecta projected onto a 2D problem mesh

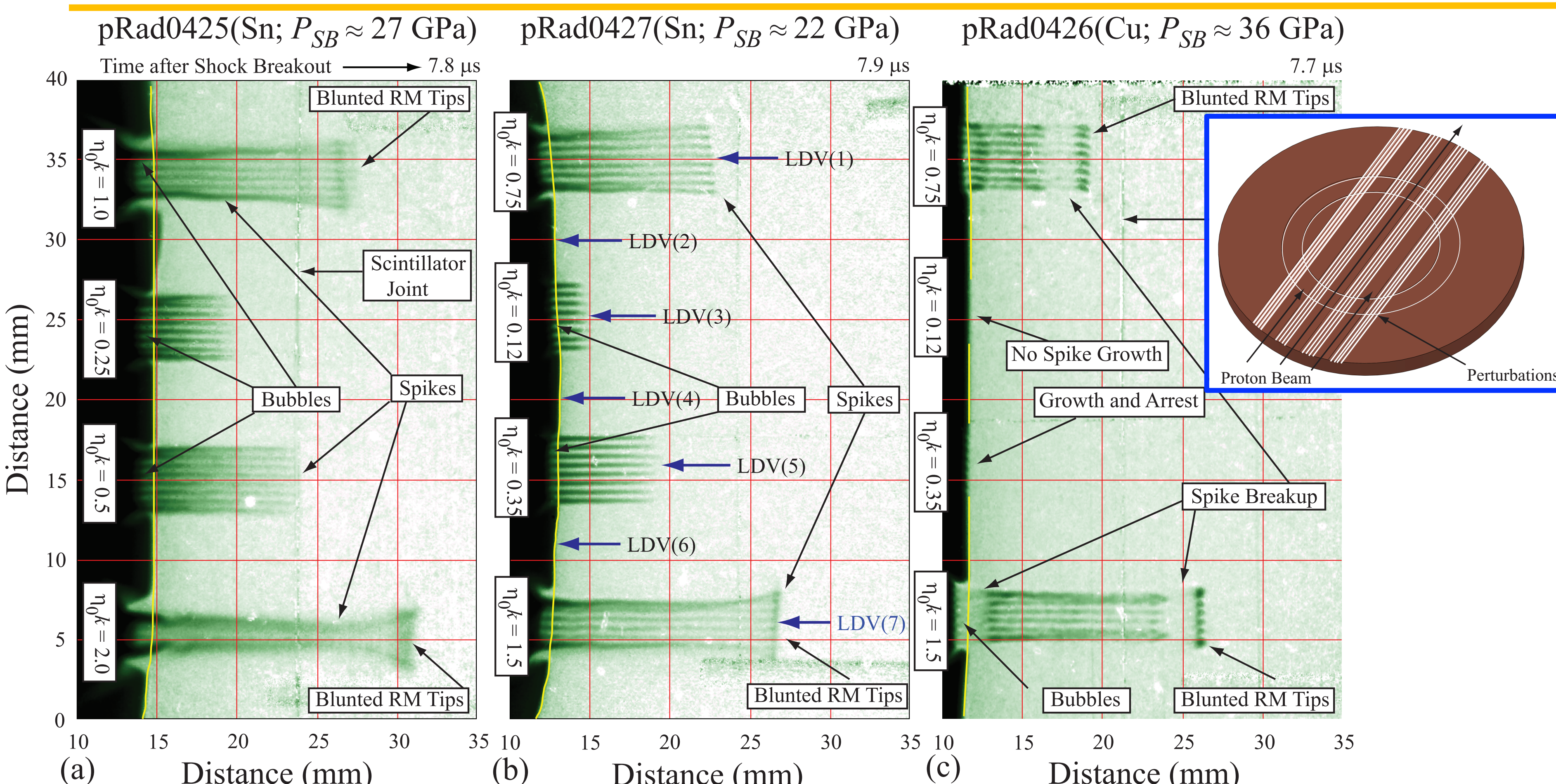


Ejecta on a 3D problem mesh

The ejecta package in FLAG is modular, with models corresponding to different stages of ejecta development

- Source models determine *whether/when* to produce ejecta, the *production amount (or rate)*, and the *initial conditions* (size and velocity distributions) of the particles produced
  - The production decision is based on shock detection and surface properties
  - “Prescriptive” source models allow the user to specify the production rate
  - “Predictive” (physics-based) models, including the Richtmyer-Meshkov Instability (RMI) model, predict the production rate or amount
  - Size and velocity distributions are specified by the user*
- Transport models account for interactions between particles and the surrounding gas
  - The user may select a drag model
  - The user may enable pressure-based (buoyant) forces on the particles
  - The Taylor Analogy Breakup (TAB) model (to be described) is a new particle breakup model
  - *We hope to combine RMI, drag and TAB models to eliminate the need for user-specified distributions

Under conditions known to produce ejecta, proton radiography shows the spikes and bubble of RM instability



W. T. Buttler, D. M. Oró, D. L. Preston, K. O. Mikaelian, F. J. Cherne, R. S. Hixson, F. G. Mariam, C. Morris, J. B. Stone, G. Terrones and D. Tupa, Journal of Fluid Mechanics **703**(July 2012):60-84
DOI: 10.1017/jfm.2012.190, Published online: 13 June 2012

Ejecta particles are droplets broken off spike tips

Buttler *et al.* (2012) analysis of spike and bubble growth rates (based on earlier work by Mikaelian):

$$\dot{\eta}^b(t) = \frac{2\dot{\eta}_0^b}{2 + 3\dot{\eta}_0^b kt} \qquad \dot{\eta}^s(t) \simeq \sqrt{3}\,\dot{\eta}_0^s$$

with initial rates

$$\dot{\eta}_0^{b,s} = \pm F_l\, F_{nl}^{b,s}\, a\, u_{fs}$$

where

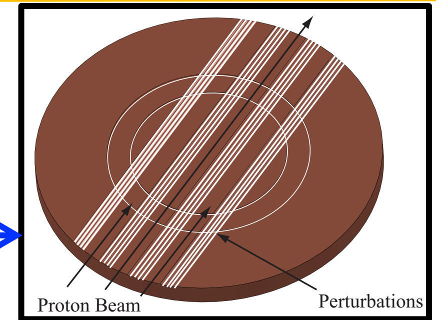
$$a = \eta_0 k = \frac{2\pi\eta_0}{\lambda} \qquad F_l = 1 - \frac{u_{fs}}{2u_{sh}}$$

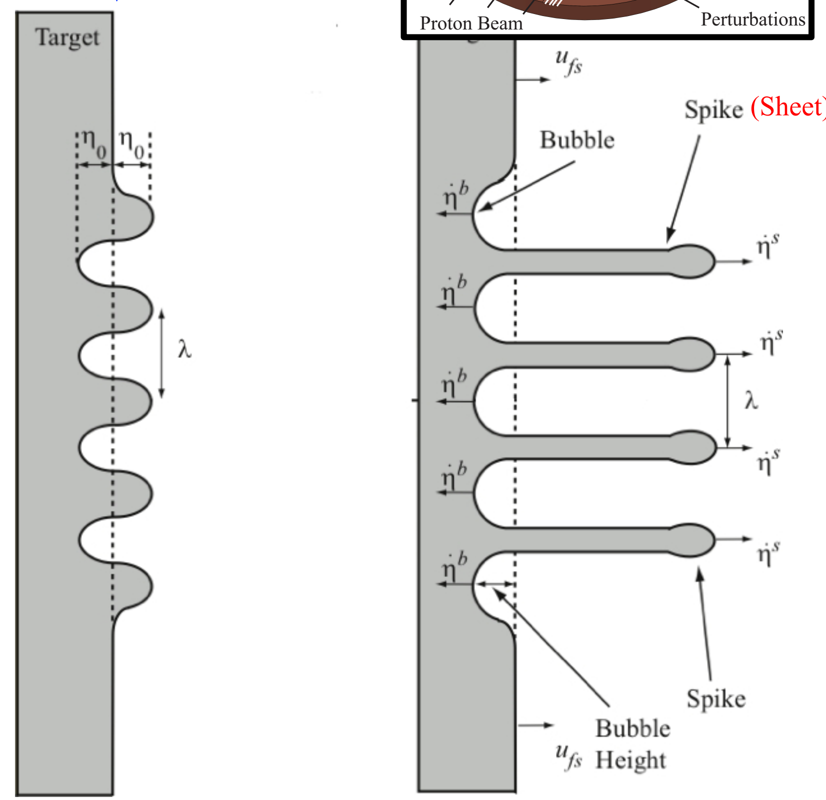
$$F_{nl}^b = \frac{1}{1 + \frac{a}{6}} \qquad F_{nl}^s = \frac{1}{1 + \frac{a^2}{4}}$$

u_{sh} = shock velocity

u_{fs} = free surface velocity

side view of this





Ejecta production rate (volume/area/time) is inferred from equality of spike and bubble volumes

$$\chi_{s,b} = \text{spike, bubble area fractions}$$

$$\chi_s + \chi_b = 1$$

Spikes and bubbles must have equal growth rates:

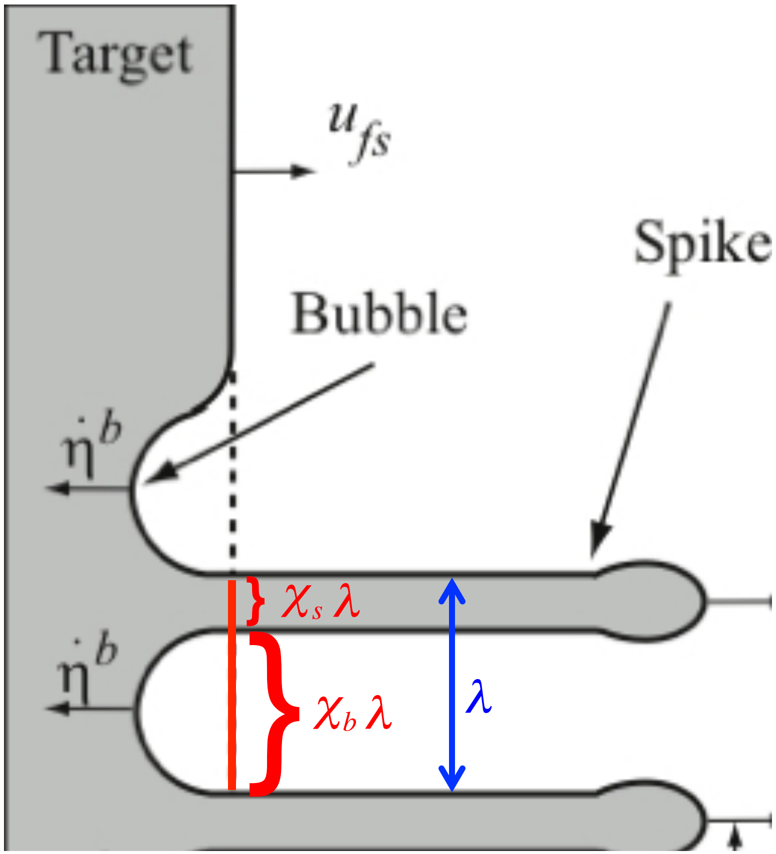
$$\dot{\Delta} = \chi_s |\dot{\eta}_s| = \chi_b \dot{\eta}_b$$

Eliminate $\chi_{s,b}$ from equations:

$$\frac{1}{\dot{\Delta}} = \frac{1}{\dot{\eta}_b} + \frac{1}{|\dot{\eta}_s|}$$

Integrate $\dot{\Delta}$ over one cycle from t_f to t_i (measured from shock breakout time):

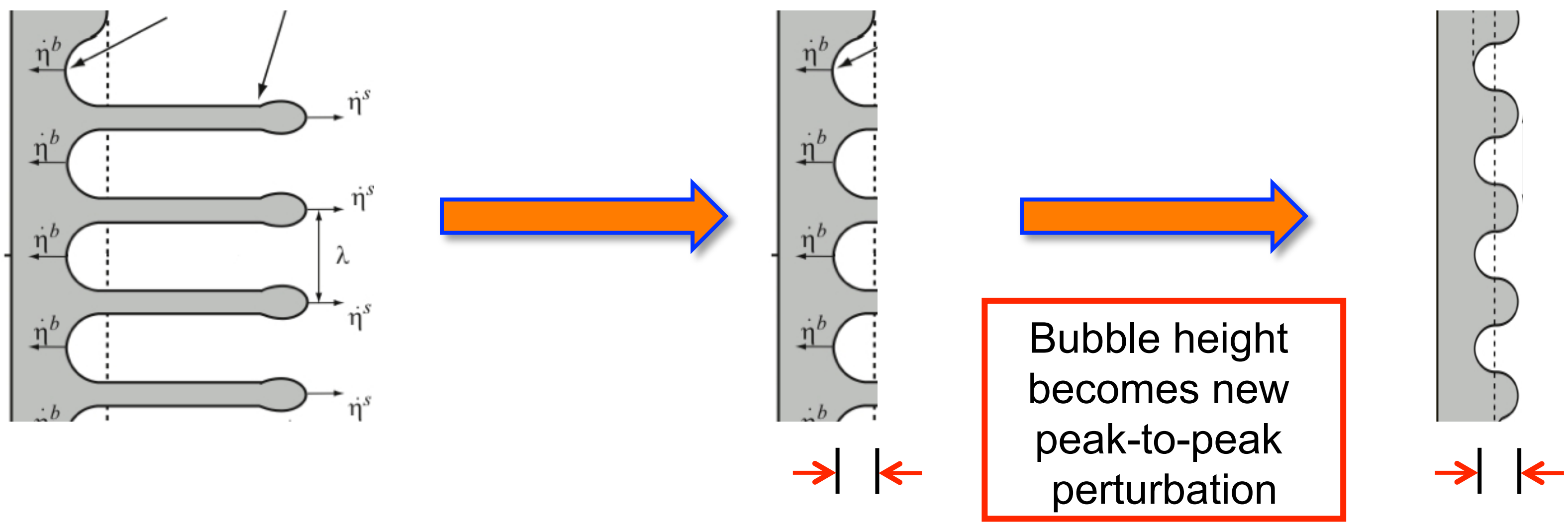
$$\Delta = \frac{2}{3k} \ln \frac{t_f + t_0}{t_i + t_0} \qquad t_0 = \frac{\frac{1}{F_{nl}^b} + \frac{1}{\sqrt{3}\, F_{nl}^s}}{\frac{3}{2} k a F_l u_{fs}}$$



The same RMI source coding is applied to second (and subsequent) shocks

We assume that spikes resulting from first shock have pinched off to form ejecta

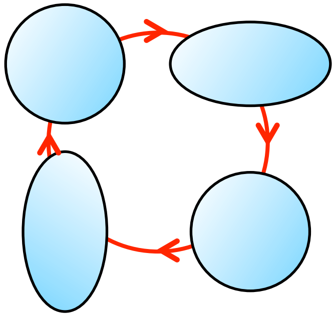
Then the bubbles provide the initial perturbation for the second shock



The rest of the analysis is unchanged

We model oscillations in a liquid droplet as a damped driven harmonic oscillator—an analogy

- Experimental evidence suggests that ejecta are liquid drops, not solid particles
- Accordingly, we have implemented a drop breakup model—the Taylor Analogy Breakup (TAB) model—in FLAG.
- We model an ejecta particle as a liquid drop
  - with radius r, density ρ_l, viscosity μ_l, surface tension σ
  - moving through a gas of density ρ_g
  - with relative velocity u



- The displacement x of the droplet's equator from its equilibrium position satisfies the differential equation

$$m\ddot{x} = F - kx - d\dot{x}$$

in which aerodynamics, surface tension and droplet viscosity provide the force terms:

$$\frac{F}{m} = C_F \frac{\rho_g u^2}{\rho_l r} \qquad \frac{k}{m} = C_k \frac{\sigma}{\rho_l r^3} \qquad \frac{d}{m} = C_d \frac{\mu_l}{\rho_l r^2}$$

Peter J. O'Rourke and Anthony A. Amsden, "The TAB Method for Numerical Calculation of Spray Droplet Breakup," LA-UR-87-2105 (revised), 1987

Solution of the damped driven harmonic oscillator

- Suppose the droplet breaks up when $x = C_b\, r$, and define $y = \dfrac{x}{C_b\, r}$. Then the solution of the ODE is

$$y(t) = C_0\,\mathrm{We} + e^{-t/t_d}\left\{(y_0 - C_0\,\mathrm{We})\cos\omega t + \frac{1}{\omega}\left[\dot{y}_0 + \frac{1}{t_d}(y_0 - C_0\,\mathrm{We})\right]\sin\omega t\right\}$$

in which

$$C_0 = \frac{C_F}{C_b\, C_k} \qquad \mathrm{We} = \frac{\rho_g\, u^2\, r}{\sigma}$$

$$\frac{1}{t_d} = \frac{C_d}{2}\frac{\mu_l}{\rho_l\, r^2} \qquad \omega^2 = C_k\frac{\sigma}{\rho_l\, r^3} - \frac{1}{t_d^2}$$

($\omega^2 < 0$ only for very small drops)

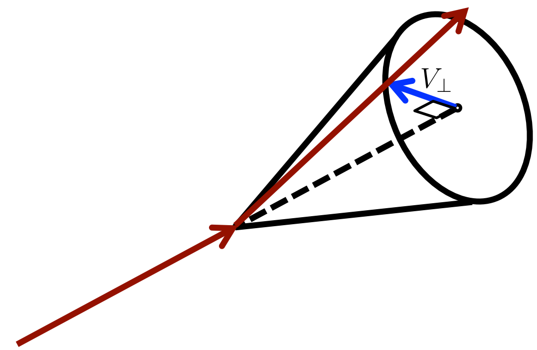
- Default coefficient values are based on experiments and modeling hypotheses:

$$C_k = 8 \qquad C_d = 5 \qquad C_b = \frac{1}{2} \qquad C_F = \frac{1}{3} \qquad C_0 = \frac{1}{12} = \frac{1}{2\,\mathrm{We}_{\mathrm{crit}}}$$

- At every cycle, for each particle, FLAG updates y and $\dot{y}$ and checks for the breakup condition $|y| = 1$.

Whenever a particle breaks up (y = 1), we must model the daughter droplets

- Daughter droplets acquire a new velocity increment perpendicular to the original velocity vector



$$V_\perp = C_v \, \dot{x}|_{t=t_{bu}} = C_v \, C_b \, r \dot{y} \qquad \text{(default } C_v = 1\text{)}$$

- An energy conservation argument determines the Sauter mean radius $r_{32} \equiv \langle r^3 \rangle / \langle r^2 \rangle$ of the expected distribution of daughter droplet radii:

$$r_{32} = r \left[1 + \frac{2K}{5} + \left(\frac{K}{20} - \frac{1}{24} \right) \frac{\rho_l \, r^3 \dot{y}^2}{\sigma} \right]^{-1} \qquad \text{(default } K = 10/3\text{)}$$

  - It suffices to create a single daughter, with the direction of $V_\perp$ sampled from [0,2π], and radius sampled from the indicated size distribution
  - We must rescale the number of physical particles in the daughter packet

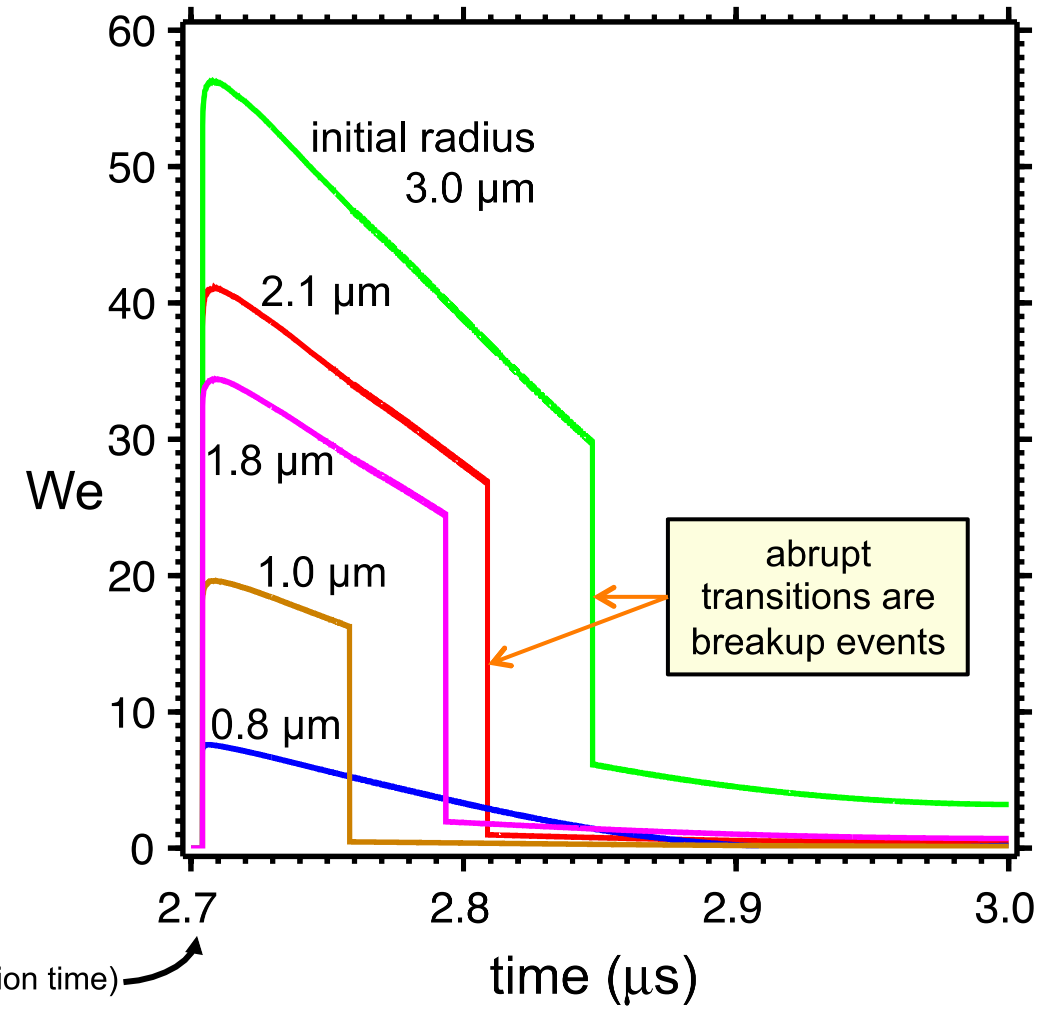
$$N^{\text{new}} = N \left(\frac{r}{r^{\text{new}}} \right)^3$$

  - Since the parent particle is replaced by the daughter in a calculation, discontinuities in time-history plots (following slides) correspond to breakup events

Particles with large Weber number break up; those with $We < We_{crit} \cong 6$ are stable

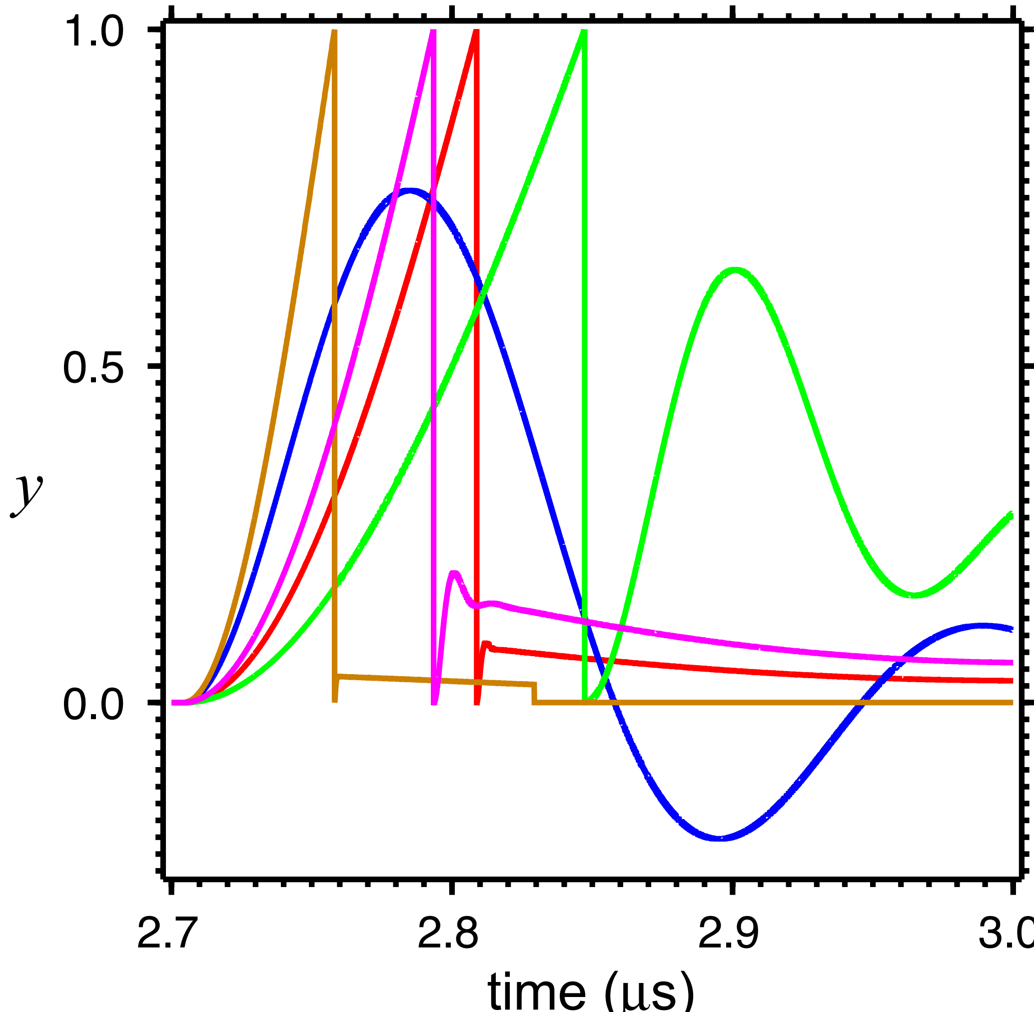
We follow five representative particles from the same simulation

$$\mathrm{We} = \frac{\rho_g\, u^2\, r}{\sigma}$$



FLAG's solution of the TAB differential equation fits the expected behavior of a damped driven harmonic oscillator

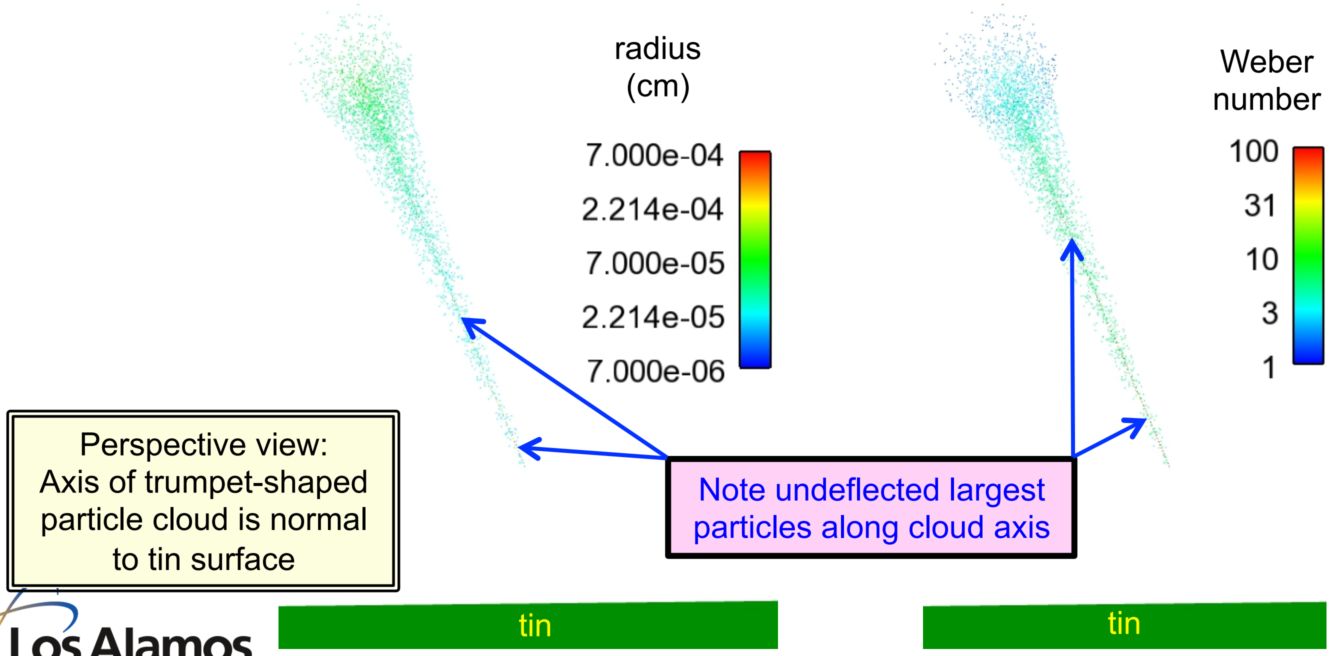
We follow the same five representative particles



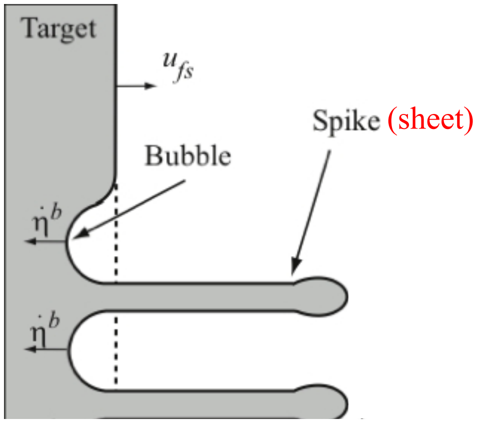
$|y| = 1$ is breakup criterion

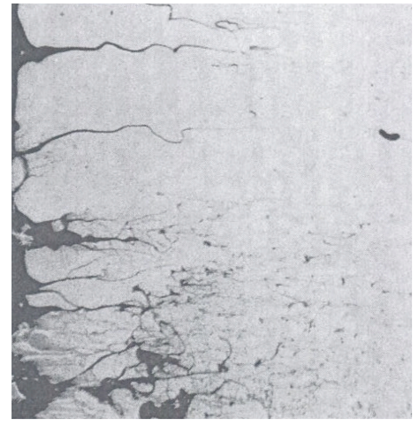
A verification calculation shows the expected breakup and spreading due to the TAB model

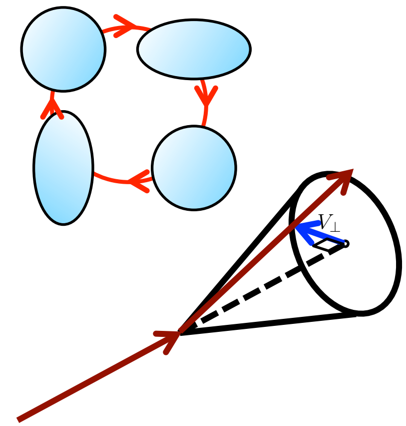
- In this artificial problem, particles were all ejected from the same point, in the same direction, with equal densities and speeds and a distribution of masses (and radii)
- Particles that broke up were given lateral velocity increments
- Particles not yet broken up are not deflected



We plan to account for the entire sequence of phenomena, between the RMI and TAB models







RMI source model: production of sheets → TAB-SHEET model (under development): sheets tear into ligaments → TAB-LIG model (under development): ligaments break up into droplets → TAB model: droplets break up into smaller droplets

The TAB-SHEET and TAB-LIB models have been developed recently* and will soon be implemented in FLAG

*M. J. Andrews and D. L. Preston, “TAB models for liquid sheet and ligament breakup,” private communication

Summary: current status and future plans

- The Richtmyer-Meshkov Instability (RMI) source model is operating and being validated for first and subsequent shocks
- The Taylor Analogy Breakup (TAB) transport model is implemented and undergoing verification calculations
- We hope to validate the TAB model in the near future
- LANL theorists have extended the TAB model to breakup of sheets and ligaments
- We plan to integrate all these pieces into a framework describing phenomena from the shocked surface to small (sub-$\mathrm{We}_{\mathrm{crit}}$) droplets

Acknowledgments

- We acknowledge collaborations, discussions and support from Malcolm Andrews, Billy Buttler, Frank Cherne, Jimmy Fung, Jim Hammerberg, Russ Olson, Dean Preston, Matthew Williams and the FLAG development team.
- This work was supported by the NNSA's ASC program.

Backup slides

The first step in source modeling is the decision whether to produce ejecta at a given mesh face, at a given time

- Ejecta particle generation is triggered when the surface acceleration exceeds some user-specified threshold $a_{threshold}$
- The threshold may optionally be decreased if the material is damaged, melted, etc.

$$\tilde{a}_{threshold} = \frac{a_{threshold}}{1+\sum c_n S_n}$$

$c_n =$ user-settable coefficients
$S_n =$ variables for damage, failure, melt, porosity $(0 \le S_n \le 1)$

For instance, if S_1 is the melt flag ($S_1 = 1$ where material is melted), then setting $c_1 = 9$ will depress the threshold by a factor of 10 wherever the surface is melted

- Two triggering options are available:
  - begin mass ejection as soon as acceleration exceeds threshold
  - recognize and integrate shock profile, then begin ejection as soon as shock passes

The second option is used for the RMI source model, because it depends on shock properties (u_{sh}, u_{fs}) that are not known until the shock has passed

TAB verification problem input parameters

- Gas (ejecta acceptor) material:
  - gamma-law gas
  - $\gamma = 7/5$
  - $\rho = 0.01$ g/cm^3
- Target (ejecta source) material:
  - Tin at STP
  - $\sigma = 550$ dyn/cm
  - $\mu = 10^5$ poise
- Particle characteristics:
  - Velocity 1 mm/μs (in frame of free surface)
  - Mass exponentially distributed, mean 10^{-9} g