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Title: Survey of Ejecta Source Modeling in FLAG

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Survey of Ejecta Source Modeling in FLAG

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XCP-1

Ejecta Working Group meeting

August 17, 2015

Outline

- Acknowledgments
- Scope of the “ejecta source” package
- Shock detection and characterization
- Mass ejection rates inferred from (multiple) Richtmyer-Meshkov Instability (RMI) models
- Estimating ejecta particle initial sizes and velocities from the RMI model
- References

I acknowledge contributions with many colleagues
(regarding ejecta source issues—with transport etc., the list would be longer)

- Implementation—FLAG
  - Don Burton
  - Nick Denissen
  - Jimmy Fung
  - Jim Hill
  - other LAP code team
- Modeling—shock profiling
  - Ben Magolan
  - Eric Nelson
  - Brian O'Neill
  - Scott Runnels
- Modeling—RMI source
  - Malcolm Andrews
  - Billy Buttler
  - Frank Cherne
  - Guy Dimonte
  - Jim Hammerberg
  - other PEM M&B team
- Experimentalists
  - Billy Buttler
  - Russ Olson
- V&V, friendly users
  - Amy Bauer
  - Rendell Carver
  - Brent Cline
  - Shirish Chitanvis
  - Carl Hagelberg
  - Jeremy Margulies
  - Garry Maskaly
  - Leslie Sherrill
  - Steve Sterbenz
  - Guillermo Terrones
  - Ian Tregillis
  - Matt Williams
  - Tony Zocher
  - (did I miss anyone?)
- LLNL—peer review
  - Grant Bazan
  - Brandon Morgan
  - other ARES team
- Institutional support
  - ASC/IC/LAP
  - XCP-1

My terminology—to foster giving credit where it is due

- Model = an approximate, quantitative description of some phenomenon. Often expressed as one or more equations.
- Package = a (more or less) self-contained part of a computer code, intended for a single purpose or to simulate a single class of phenomena.
- Thus a model may be implemented in a code package.
- Referring to a piece of code as a model may slight the contributions of the modelers (e.g., “Alan Harrison’s ejecta model in the code”).

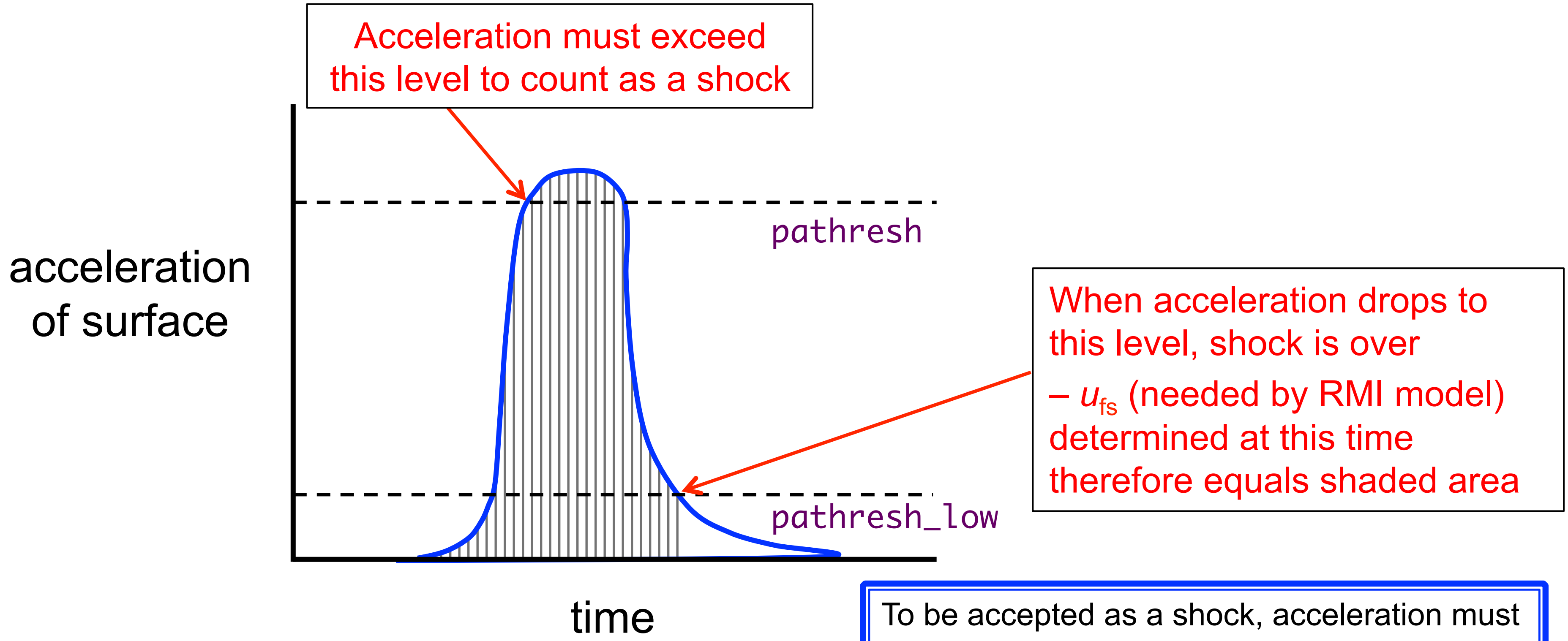
- I’m talking today about FLAG’s ejecta package, and some of the models implemented therein.

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

- The source package determines *whether/when* to produce ejecta, the *production 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 packages allow the user to specify
    - the production rate, and
    - distributions from which particle initial sizes and velocities are sampled
  - The Richtmyer-Meshkov Instability (RMI) package is "predictive," using a model of RMI to predict
    - the production rate, and
    - initial particle sizes and velocities
- Other packages account for the transport phase (including drag, pressure forces, particle breakup, and collisions*) and later events (recollection, evaporation, and hydriding*) (* = future developments)

This talk will focus on what we consider best practices for ejecta simulations with FLAG; there are other options

Shock detection and characterization is based on two acceleration thresholds

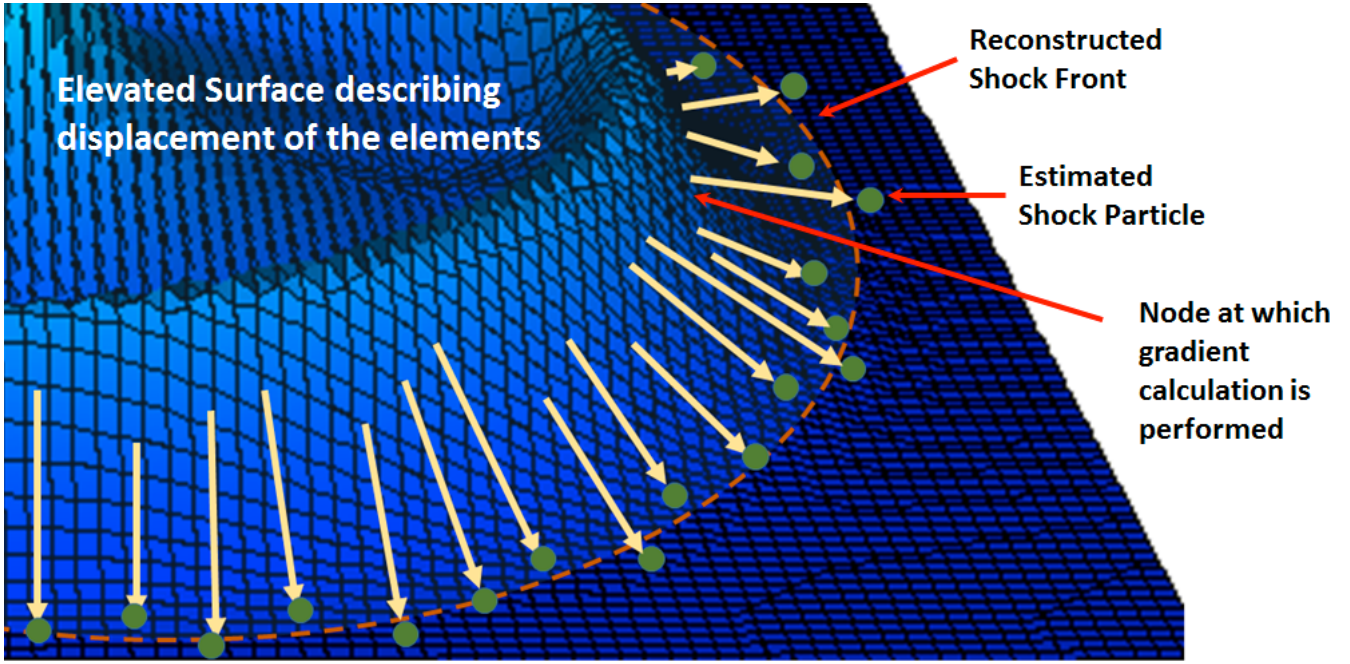


To be accepted as a shock, acceleration must
(1) start below lower threshold
(2) exceed upper threshold
(3) drop below lower threshold
and surface* must be melted at time (3)
*one zone below the surface, actually

We are exploring better methods of detecting and characterizing shocks

- Scott Runnels and I researched this with grad students Ben Magolan, Brian O’Neill in 2014

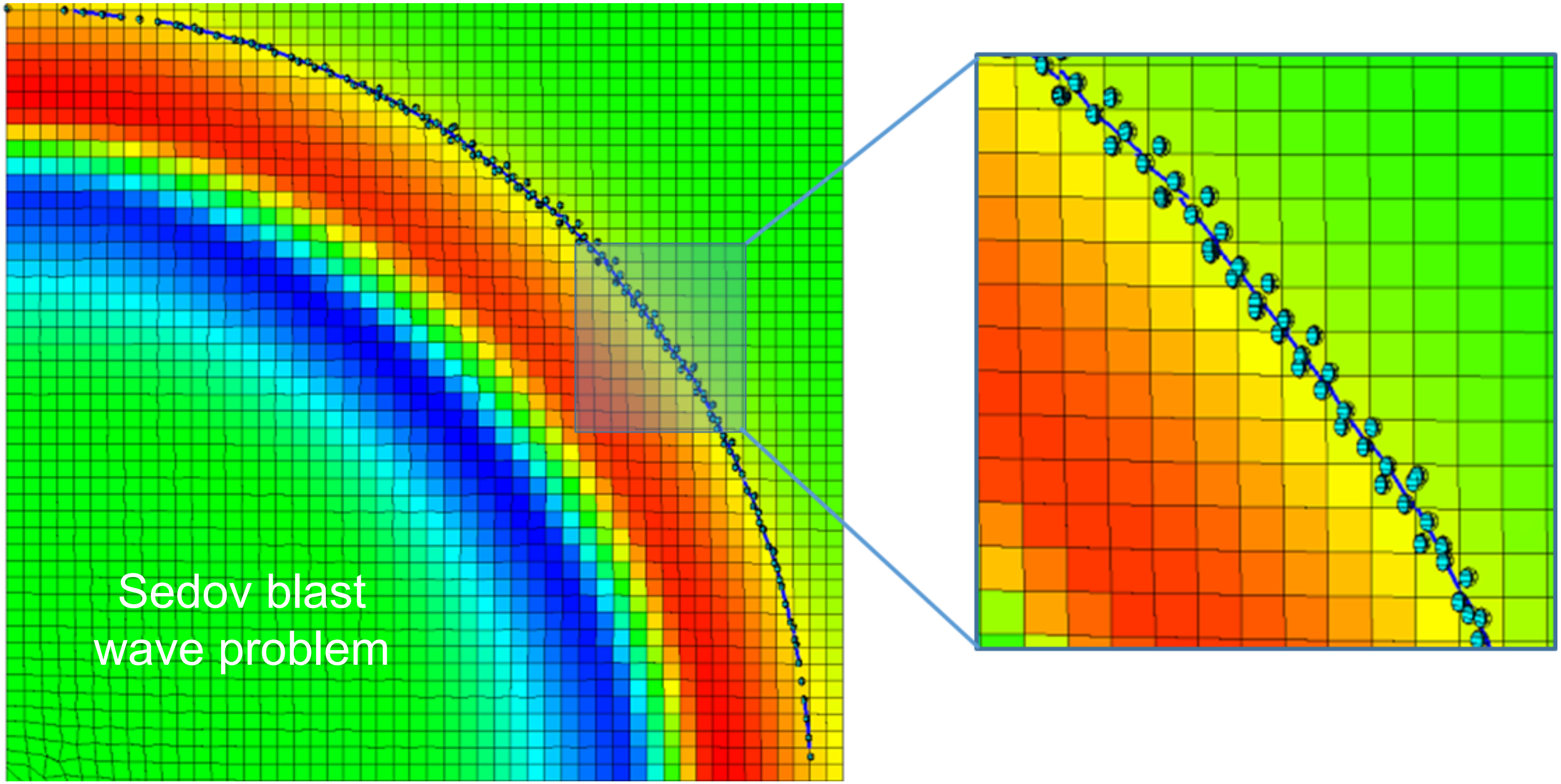
- It is based on a 1D method from Eric Nelson



- This needs further development

- It holds the promise of better estimates of u_{sh}, among other things.

The students implemented the 2D shock profiling method in FLAG



Mass ejection rate computed from RMI model:
Original form (isolution_method=0)

Buttler *et al.* (2012) equations (2.4) [Mikaelian(1998) equation (17)] and (2.3):

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

with initial rates

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

where

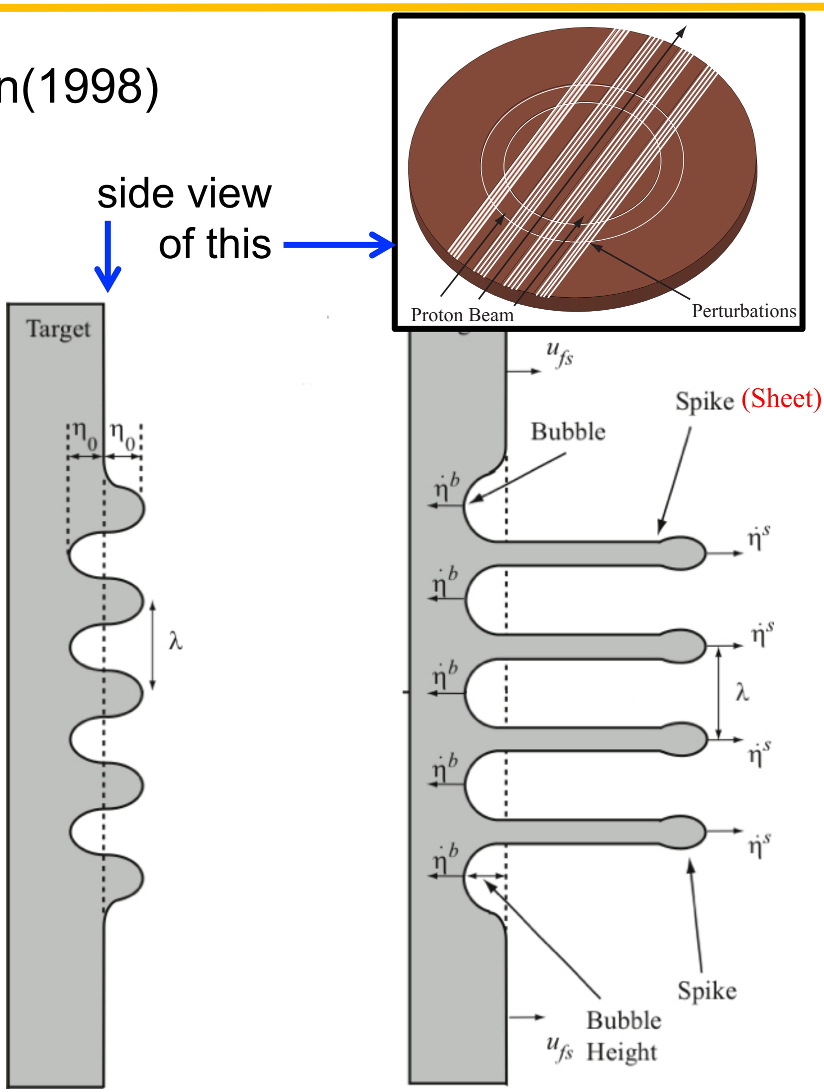
$$a = \eta_0 k = \frac{2\pi\eta_0}{\lambda} \qquad F_l = 1 - \frac{u_{fs}}{2u_{sh}}$$

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

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

$\chi_{s,b}$ = 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: $\dfrac{1}{\dot{\Delta}} = \dfrac{1}{\dot{\eta}_b} + \dfrac{1}{|\dot{\eta}_s|}$

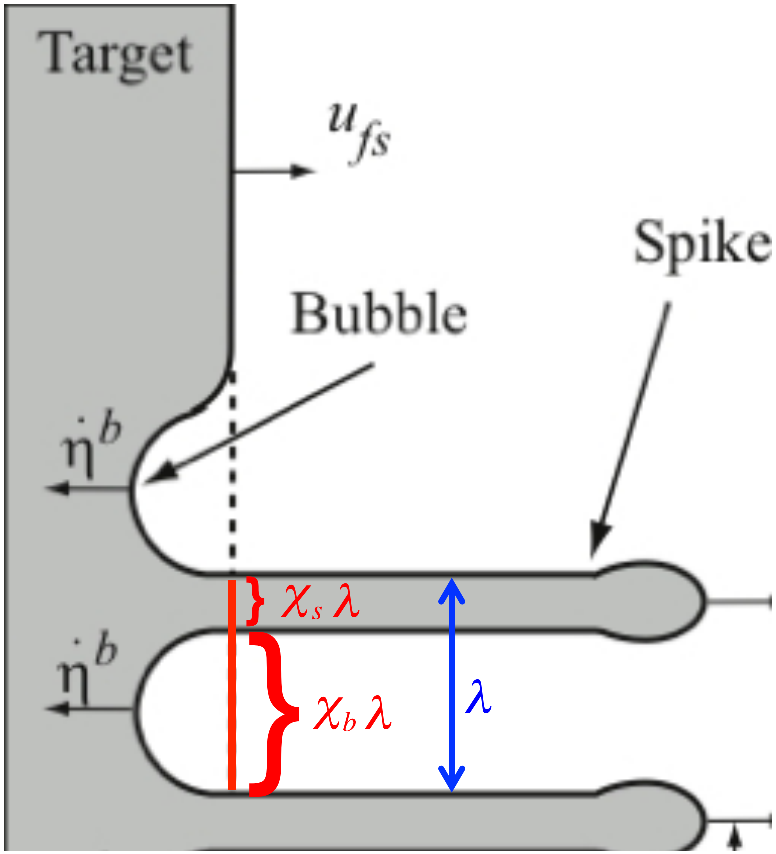
Integrate $\dot{\Delta}$ over one cycle from t_f to t_i (measured from shock breakout time):

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

which gives cumulative production equal to

$$m(t) = m_0 \ln\left(1 + \frac{t}{\beta\tau}\right)$$

in the notation of Cherne, Hammerberg *et al.*



Compare to model from Cherne, Hammerberg, Andrews, Karkhanis and Ramaprabhu (LA-UR-15-24743)

Define

$$m_0 = \frac{\rho\lambda}{3\pi} \qquad \tau = \frac{\lambda/3\pi}{F_l F_{nl}^b k \eta_0 u_{fs}} \qquad \beta = 1 + \frac{F_{nl}^b}{\sqrt{3F_{nl}^s}}$$

Then with unit shape function,

$$m(t) = m_0 \ln\left(1 + \frac{t}{\tau}\right)$$

and with (1) parabolic shape function and (2) spike/bubble volume conservation,

$$m(t) = \frac{2}{3} m_0 \ln\left(1 + \frac{t}{\beta\tau}\right)$$

compare to

$$m(t) = m_0 \ln\left(1 + \frac{t}{\beta\tau}\right)$$

in FLAG

and finally, accounting for time necessary for initial perturbation to invert,

$$m(t) = \frac{2}{3} m_0 \ln\left[1 + \frac{t - \Delta t}{(\beta + \Delta t/\tau)\tau}\right] \qquad (t \geq \Delta t)$$

Ejecta particles are droplets pinched off from spike tips: “Improved” form (isolution_method=1)

Buttler *et al.* (2012) equation (2.1)
[η_0=0 limit of Mikaelian (1998) equation (5a)]:

$$\dot{\eta}(t) = \left(\tfrac{2}{3}e^{3nk} + \tfrac{1}{3}\right)^{-1/2}\dot{\eta}_0 \qquad \dot{\eta}_0^{b,s} = \pm F_l F_{nl}^{b,s} a u_{fs}$$

where u_{sh} and u_{fs} are shock and free surface velocities

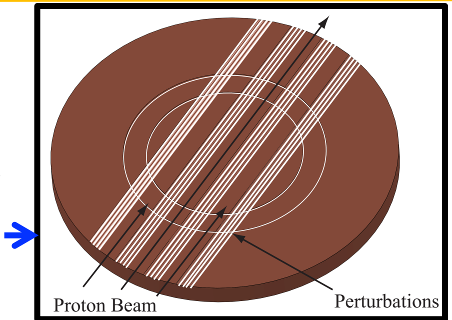
$$a = \eta_0 k = 2\pi\eta_0/\lambda \qquad F_l = 1 - u_{fs}/2u_{sh}$$

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

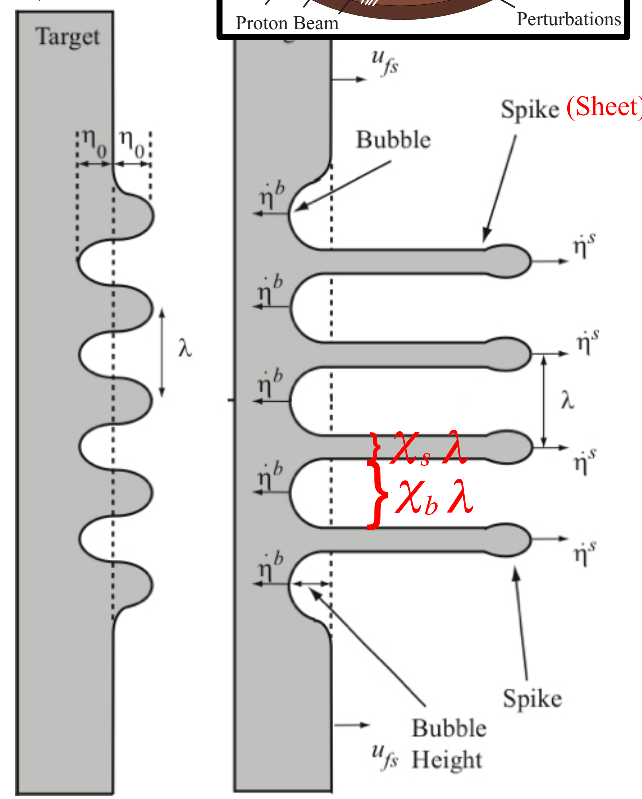
and we use equality of spike and bubble volumes

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

to find the production rate $\dot{\Delta}$.



side view of this



Timeline and genealogy of mass ejection *m(t)* forms in FLAG RMI package

Buttler *et al.* (2012) eqn. (2.4)

$$\dot{\eta}^b(t) = \frac{2\dot{\eta}_0^b}{2 + 3\dot{\eta}_0^b kt}$$

Conservation of spike/ bubble volume

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

Buttler *et al.* (2012) eqn. (2.1)

$$\dot{\eta}(t) = \left(\tfrac{2}{3}e^{3nk} + \tfrac{1}{3}\right)^{-1/2} \dot{\eta}_0$$

isolution_method = 0
Nov. 2012

$$m(t) = m_0 \ln\left(1 + \frac{t}{\beta\tau}\right)$$

2/3 factor
Hammerberg/Andrews private communication (Dec. 2014)

isolution_method = 1
Dec. 2013 (default Feb. 2014)

$$\dot{\eta}(t) = \left(\tfrac{2}{3}e^{3nk} + \tfrac{1}{3}\right)^{-1/2} \dot{\eta}_0$$

$$\dot{m}(t) = \rho\dot{\Delta} = \rho\chi_s\left|\dot{\eta}_s\right| = \rho\chi_b\dot{\eta}_b$$

isolution_method = 0
Jan. 2015

$$m(t) = \frac{2}{3} m_0 \ln\left(1 + \frac{t}{\beta\tau}\right)$$

Cherne, Hammerberg, Andrews, Karkhanis and Ramaprabhu
LA-UR-15-24743
(June 2015)

isolution_method = 1
Jan. 2015

$$\dot{\eta}(t) = \left(\tfrac{2}{3}e^{3nk} + \tfrac{1}{3}\right)^{-1/2} \dot{\eta}_0$$

$$\dot{m}(t) = \tfrac{2}{3}\rho\dot{\Delta} = \tfrac{2}{3}\rho\chi_s\left|\dot{\eta}_s\right| = \tfrac{2}{3}\rho\chi_b\dot{\eta}_b$$

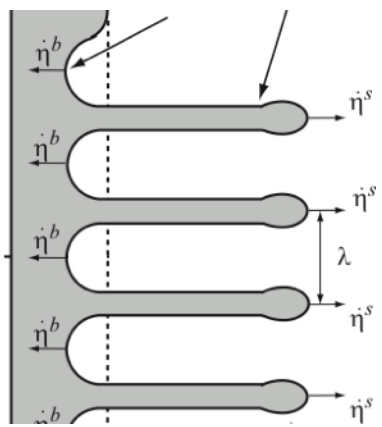
future work?

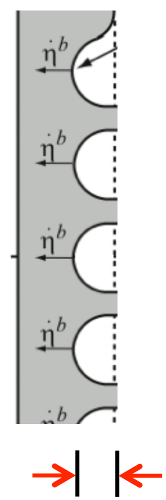
future work?

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

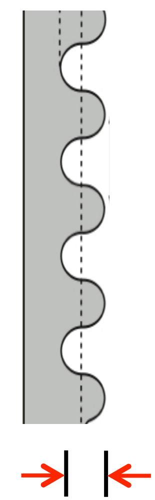
We assume that spikes resulting from first shock have pinched off to form ejecta

Then the bubbles provide the initial perturbation for the second shock





Bubble height becomes new peak-to-peak perturbation



The rest of the algorithm is unchanged

What about ejecta particle initial sizes and speeds?

- Having determined the mass ejection rate, we still need the sizes and velocities of the particles
- We use the width $\chi_s \lambda$ of the spike (at its base) as the initial diameter of the ejecta.
  - Can be quite large initially (namely, $\lambda/2$)
  - Mean width of particle cloud may drop quickly as spike thins out
  - Would a distribution of sizes be more believable?
- We use the growth rate $\dot{\eta}^s$ of the spike (at its tip) as the initial speed of the ejecta.
  - Would a distribution of speeds be more believable?

What about ejecta particle initial directions?

- We suppose that the particles are launched in a direction normal to the surface.
  - The shape and location of the resulting ejecta cloud can be very sensitive to the tilt of the mesh faces on the metal surface
  - Cherne has done some MD calculations showing a more complex picture when the shock incidence is oblique
  - Experiments…?
- All these approximations (this and the previous slide) are questionable; I would welcome some model development here.

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