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Title: Non-sinusoidal RMI Analysis and other factors

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Non-sinusoidal RMI Analysis and other factors

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General Outline

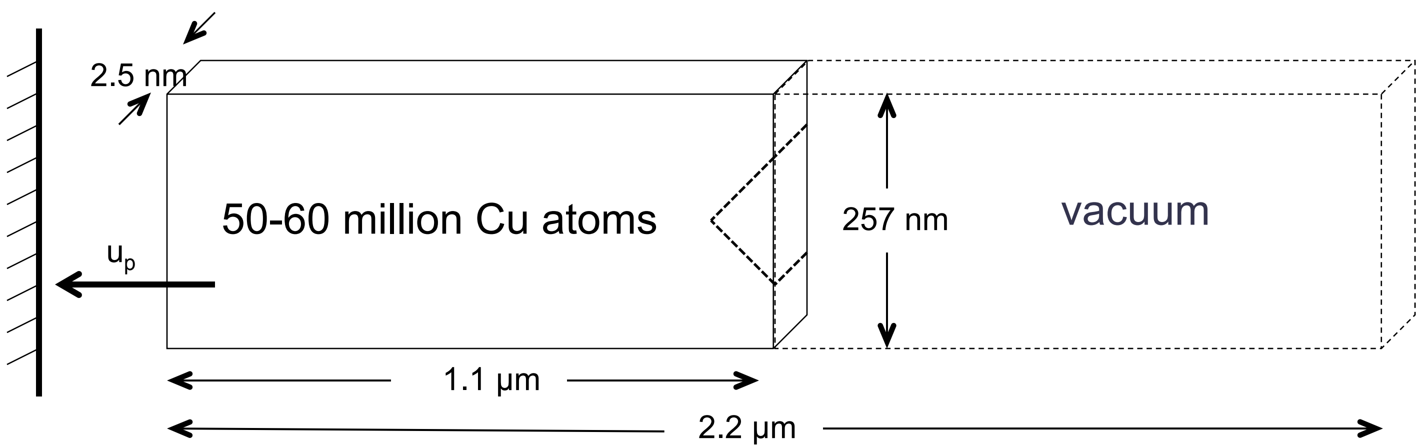
- A brief introduction as to why Molecular Dynamics over a hydrodynamic code.
- Prior molecular dynamics studies on copper looking at both sinusoidal and chevron shaped grooves.
- Present preliminary results on similar copper simulations looking the sinusoidal breakup of sheets.
- Examination of various non-sinusoidal shapes and comparing them with the ejecta model.
- Summary and Conclusions

Large-scale (>10^7-atom) molecular dynamics simulations provide insight into mechanisms

- EAM potential for Cu [A. F. Voter, PRB **57**, 13985 (1998)]

$$E_i = F\left[\sum_j \rho_j\left(r_{ij}\right)\right] + \frac{1}{2}\sum_{i\neq j}\varphi\left(r_{ij}\right)$$

- Quasi-2D geometry (periodic boundary conditions in lateral directions):



- The material properties such as surface tension and viscosity result from the potential.

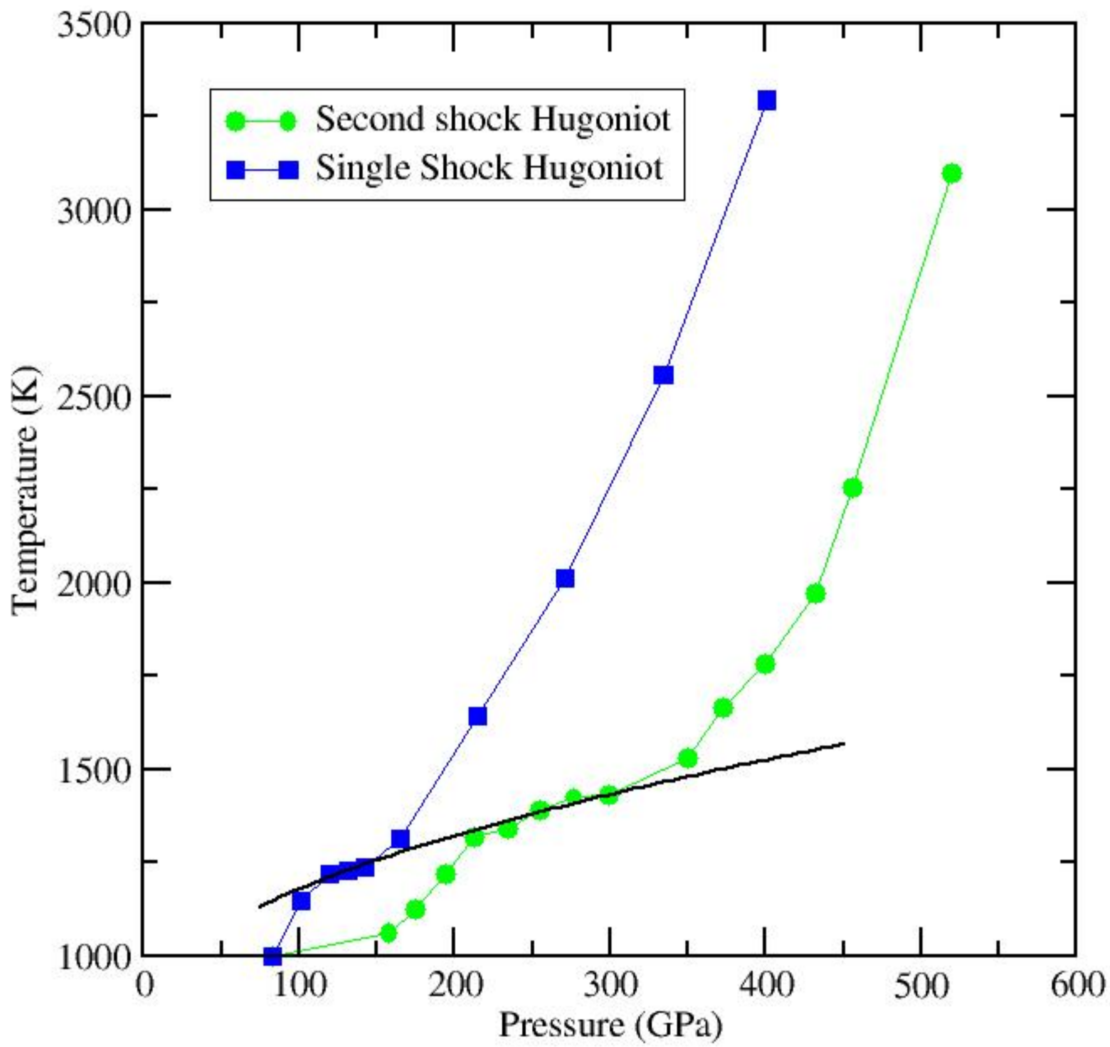
To understand the inhibition of Richtmyer-Meshkov instability growth by material strength, we have focused on single-mode geometries

- **Sinusoidal surface profile, with scaled amplitude** $kh_0 = \frac{2\pi h_0}{\lambda}$

- **An fcc lattice of atoms were oriented so that the shock wave was going down the <111> orientation.**
  - 60 million atoms
  - The dimensions of the simulated cell were 257 nm x 2.5 nm x 1100 nm
  - A sinusoidal groove of varying amplitudes were “machined” ranging from 1-41 nm

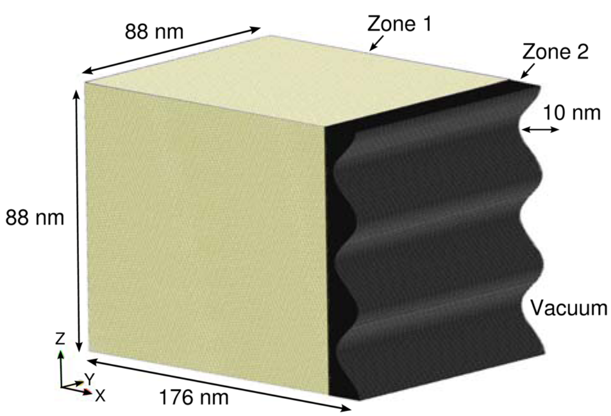
The single shock copper Hugoniot and secondary shock Hugoniot provide a clear phase boundary line

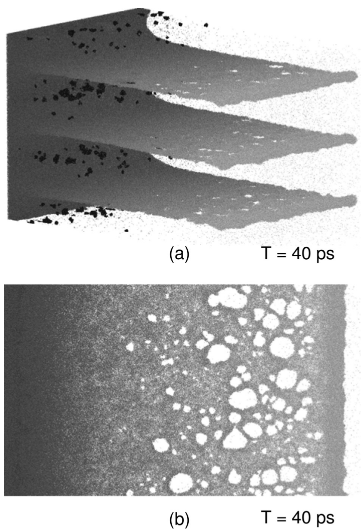
- **Creation of a double shock**
  - Instantly change the momentum of the atoms impacting the wall as a factor of the first shock strength at some time delay.
- **The mixed phase region for the single shock and double shocked state allow for the mapping of the phase boundary in copper.**



Prior works by the O. Durant and L. Soulard (JAP 111,044901 (2012)

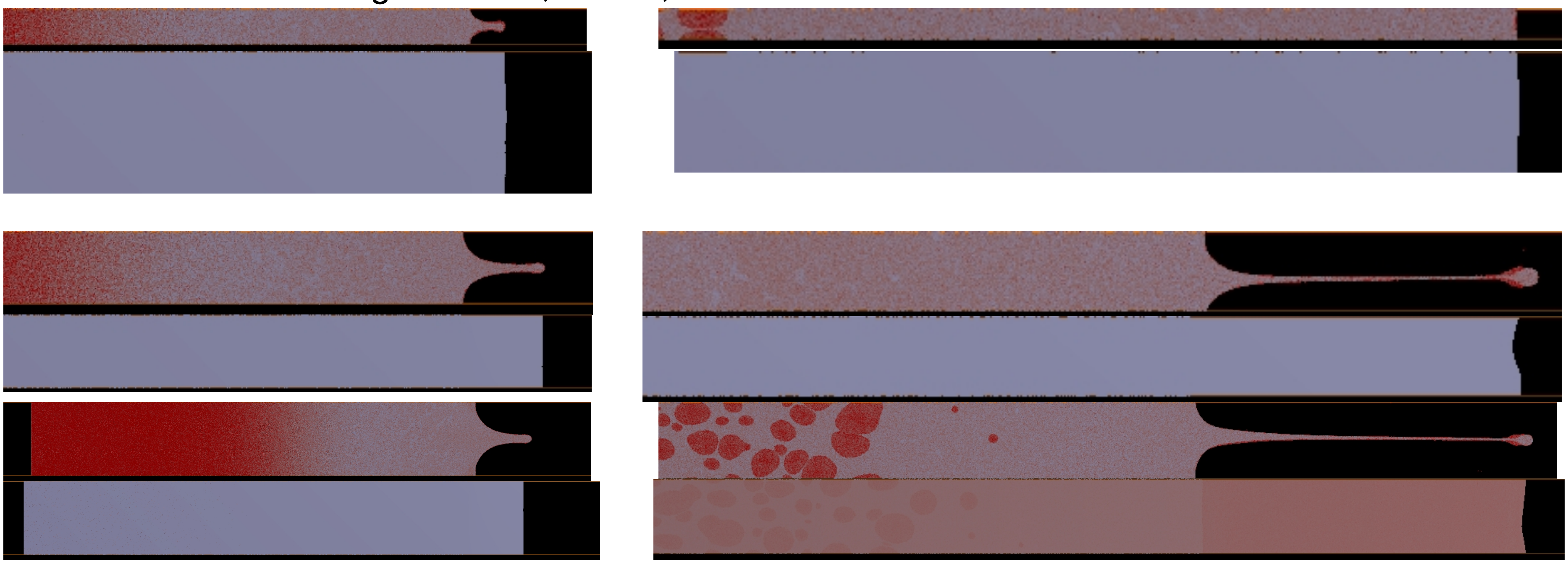
- The MD simulation sizes were typically on the order of 88 nm (3 wavelengths) x 88 nm x 176 nm (shock direction).
- Round trip transit times of the release waves provide short lived sustained shocks.
- Typical shock strength was a up of ~3.5 km/s.
- Breakup of the spikes and bubbles showed a large degree of atomization and short break up times.



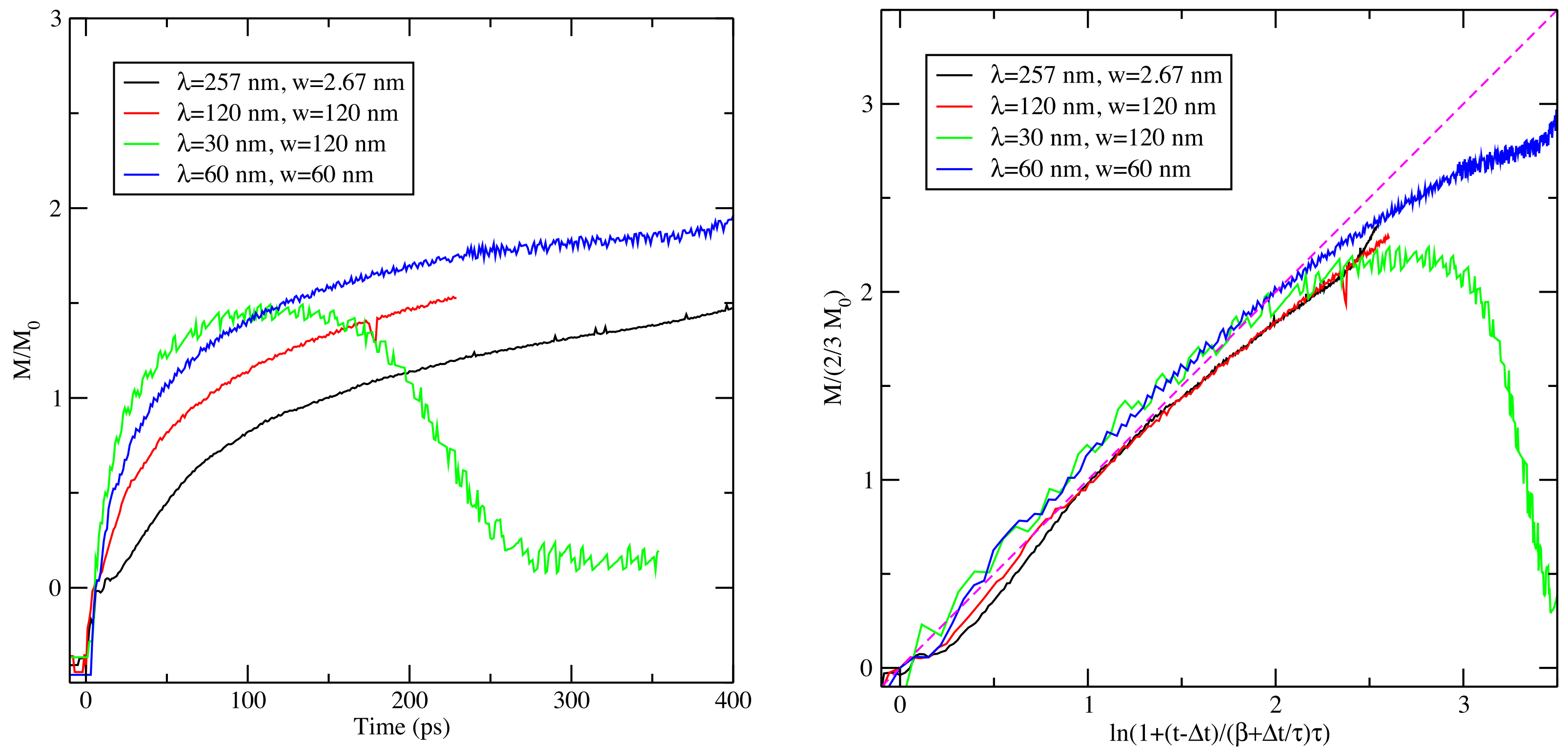


Simulations using 3 different wavelengths with a wide cross-section and a “long” shock direction length.

- **The images presented here are late time nominally the same time after shock breakout from the bottom of the surface all with a kh0=0.5 at a up=2.5 km/s.**
  - Wavelength=30 nm, 60 nm, and 120 nm



Scaled Areal Mass densities are comparable yet the 30 nm wavelength shows a recoil.

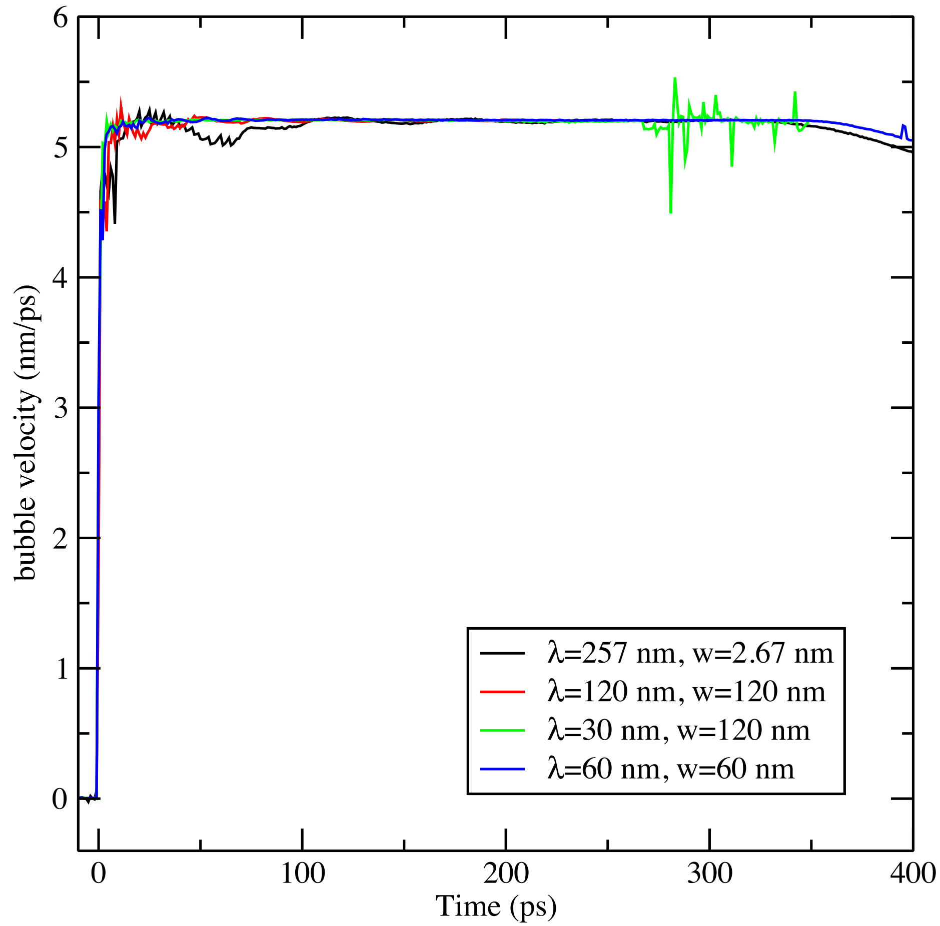


Bubble velocities for each of the wavelength and width combinations show pretty good agreement.

- Late time decay in the bubble velocity is directly related to the release wave reaching the bubble interface.

- For the wider simulations there is good agreement with a small amount of noise at early times.

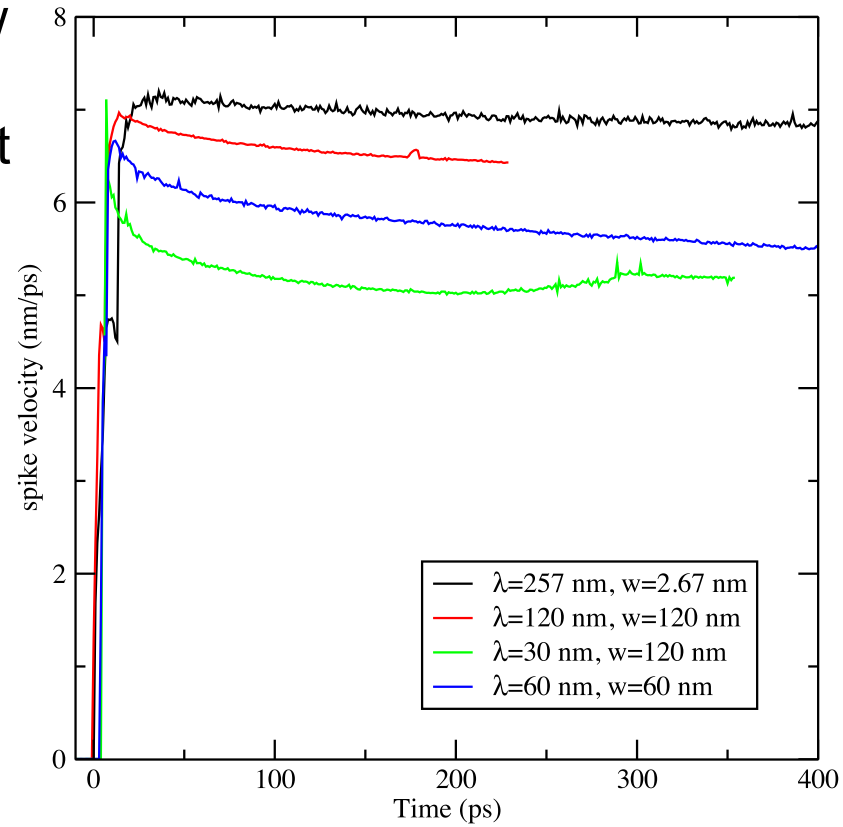
- The narrow simulation at early times shows some fluctuations in the bubble velocity.



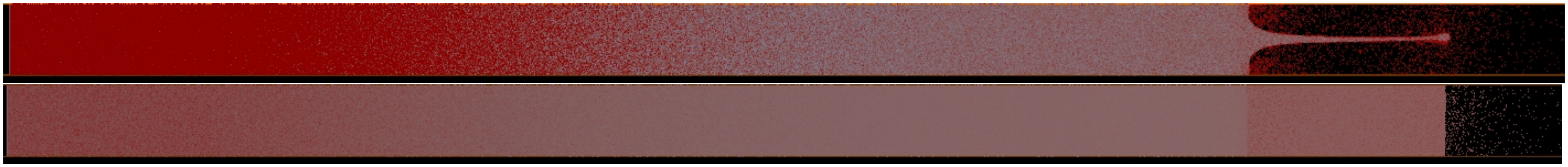
Spike velocities show a decay which could be related to viscosity or surface tension effects.

- The longest wavelength yet narrow simulation shows a slight decay in the velocity as a function of time yet is around 7 nm/ps or approximately 2 nm/ps greater than the free surface velocity.

- All the other simulations show variable decays as a function of wavelength in spite of the same value for the kh_0. The 30 nm wavelength simulation actually falls slightly below the free surface velocity.



In looking at a similar u_p value as O. Durand and L. Soulard at t=

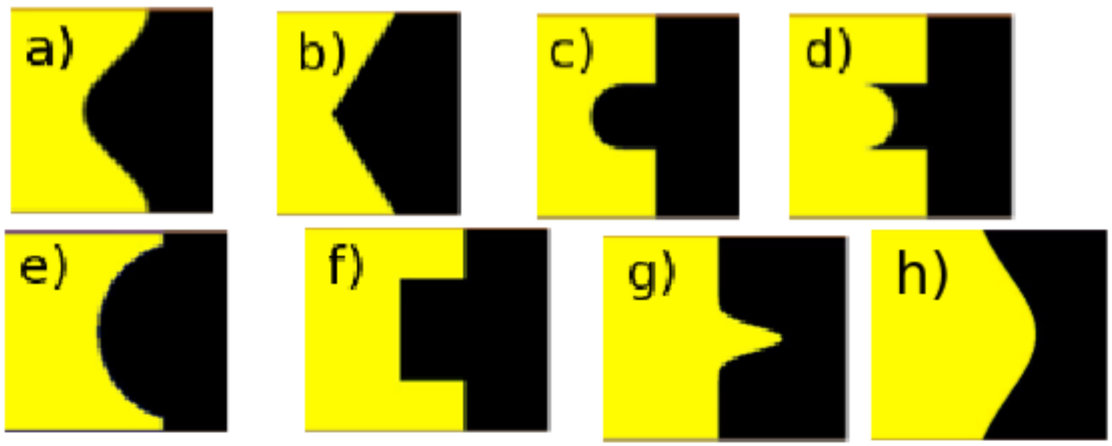


- The delta time between the upper and lower images is 36 ps which is much longer than the time where Durand observed breakup.

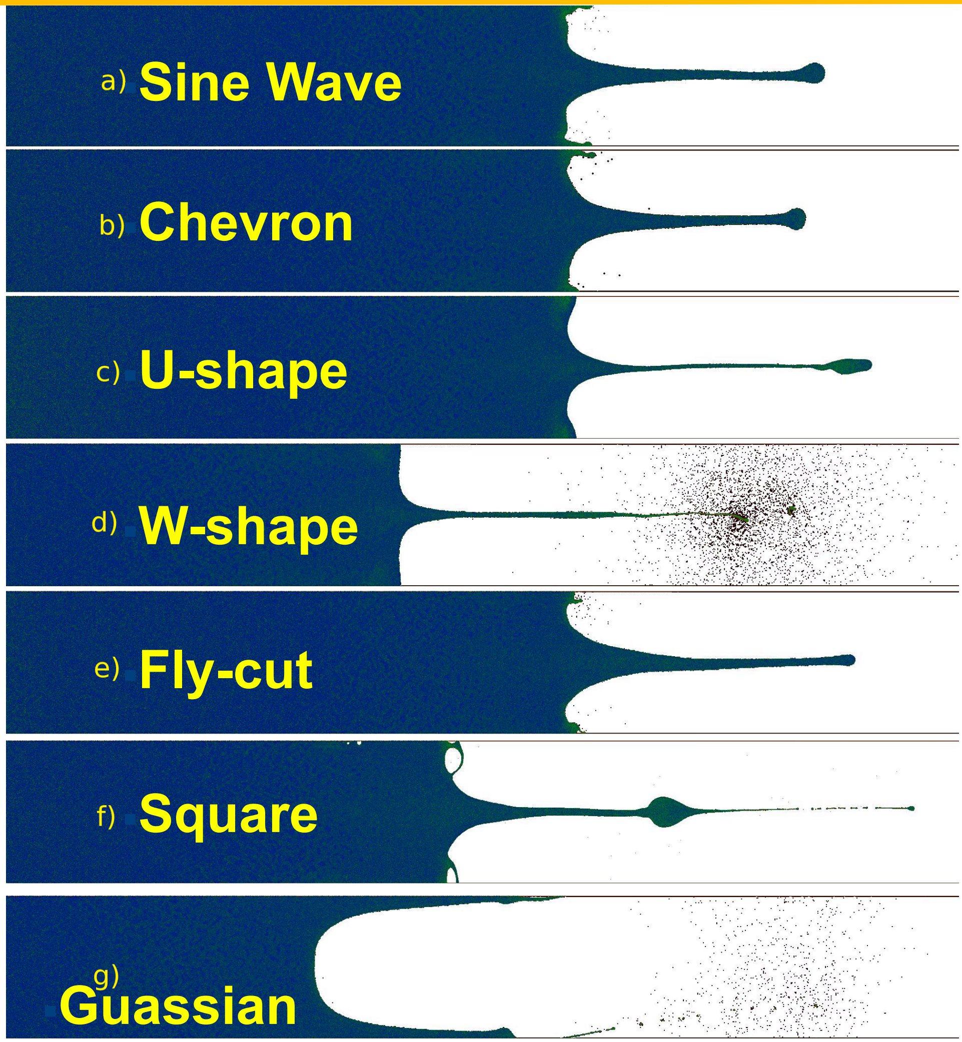
- A shorter shock direction simulation is currently underway at this shock strength to see if the void formation is percolating into the bubble region assisting in the break up of the spikes.

Examination of various surface shapes upon ejected mass

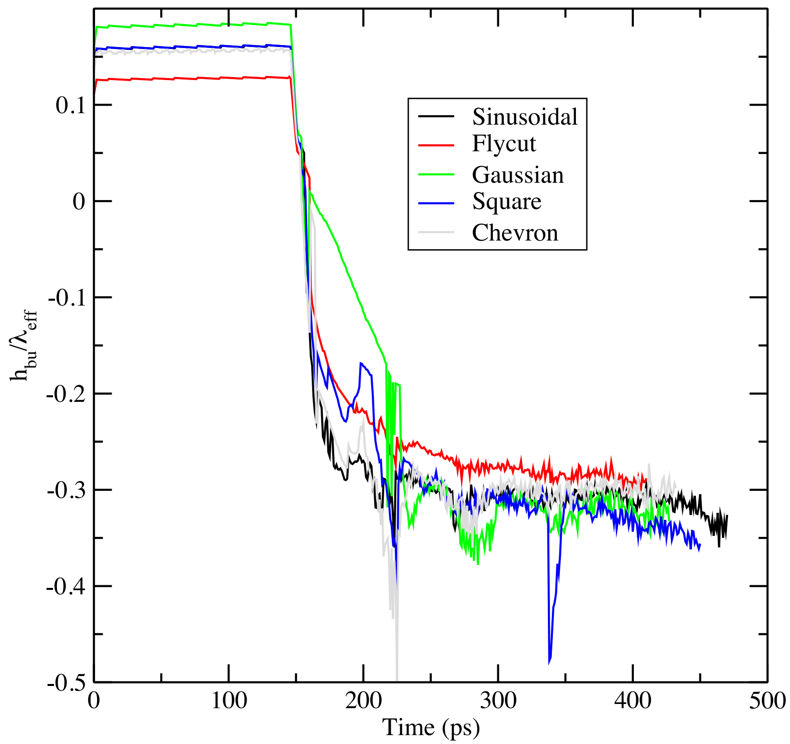
- **Examine the effect of surface profile upon ejecta formation**
- **Conditions:**
  - u_p= 2.5 km/s (material is melted upon 1st shock)
  - kh_0= 1.0
- **Shapes:**
  - Sine wave
  - Chevron
  - U-shape
  - W-shape
  - Fly-cut profile
  - Square wave
  - **Narrow Gaussian**
  - Wide Gaussian

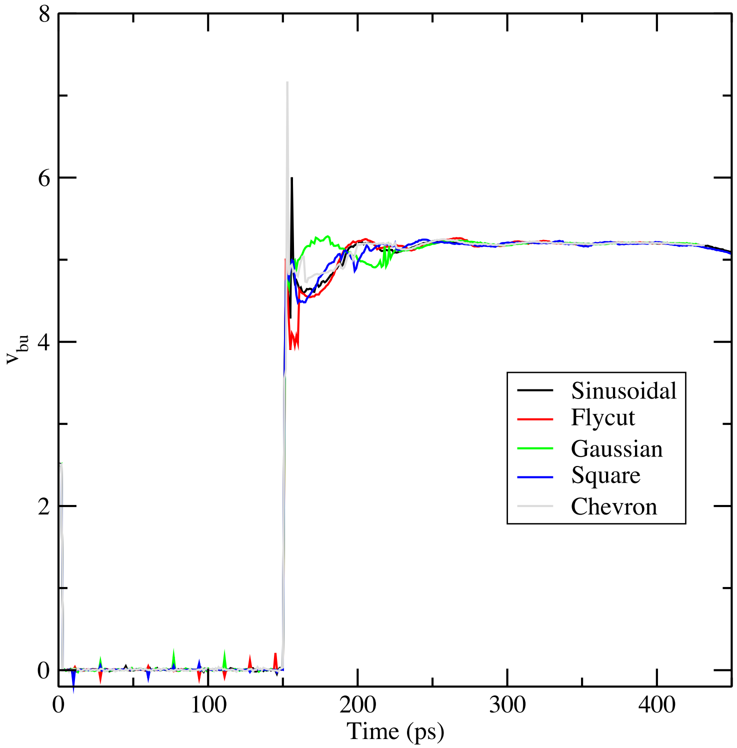


Spike tip growth for u_p=2.5 km/s as a function of shape

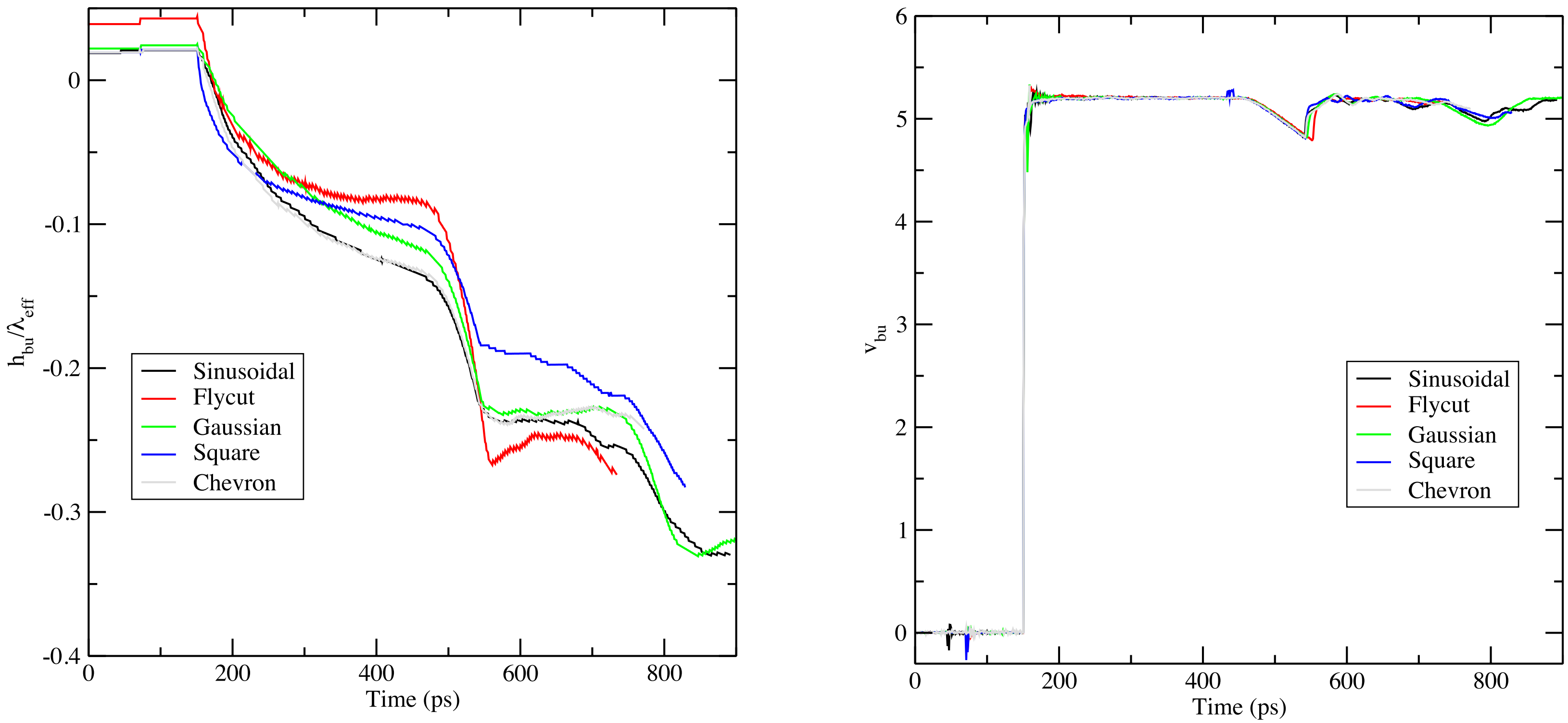


Bubble heights and velocities for kh_0=1.0

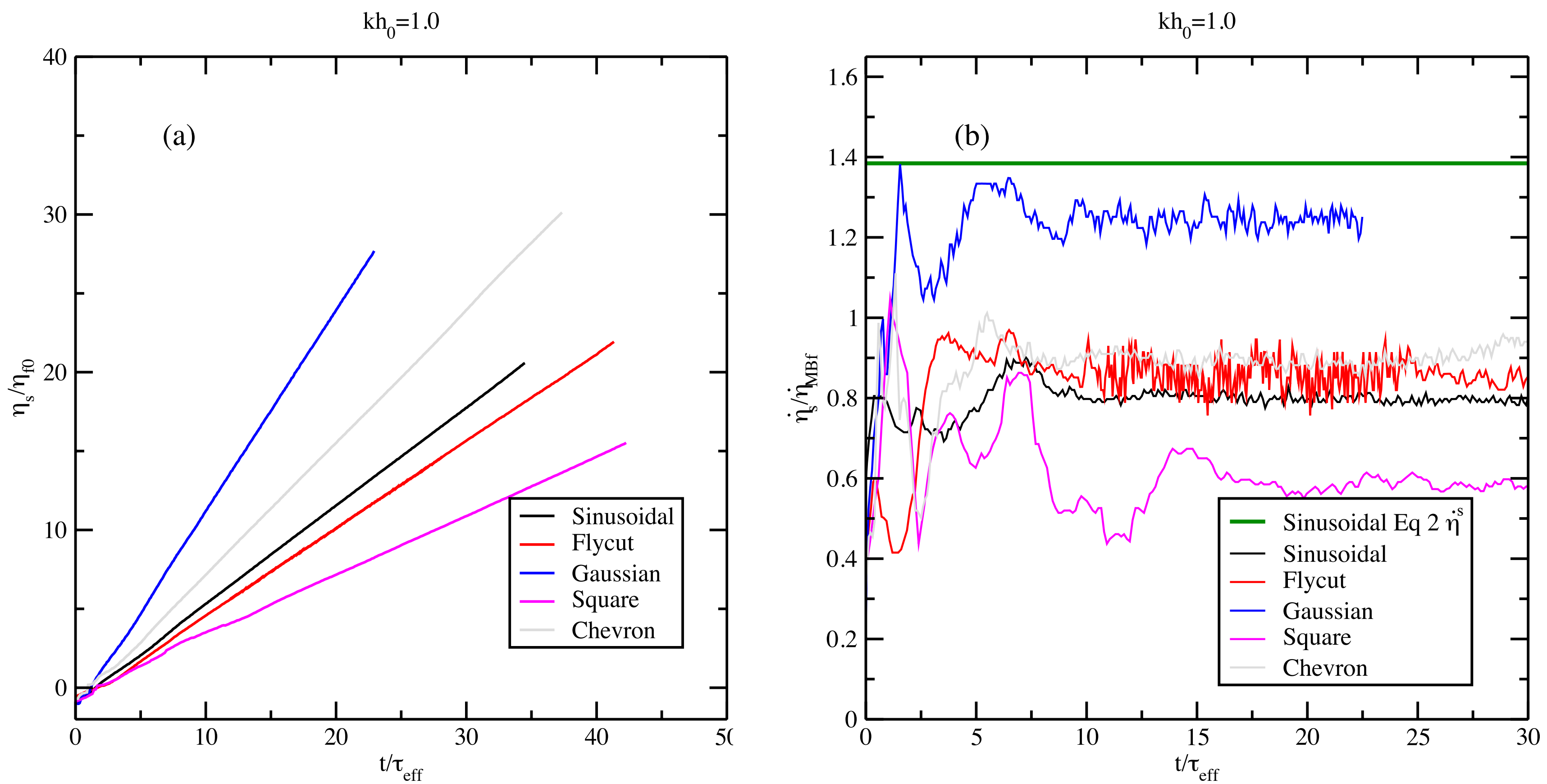




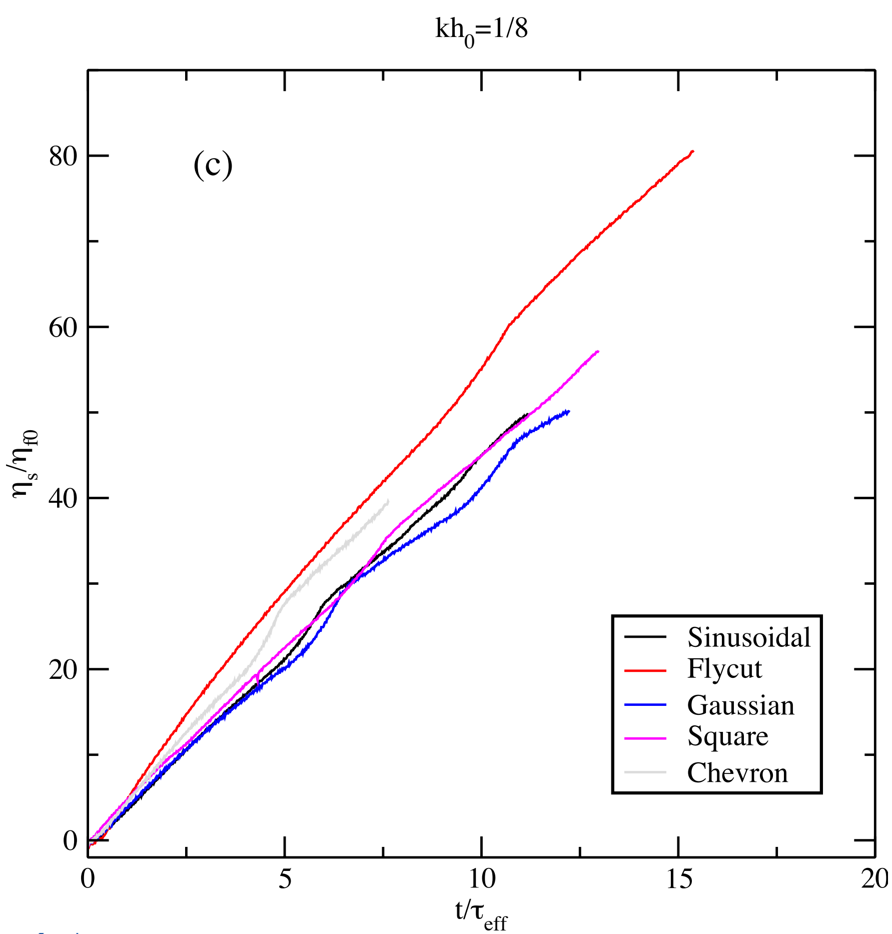
Bubble heights and velocities for kh_0=1/8

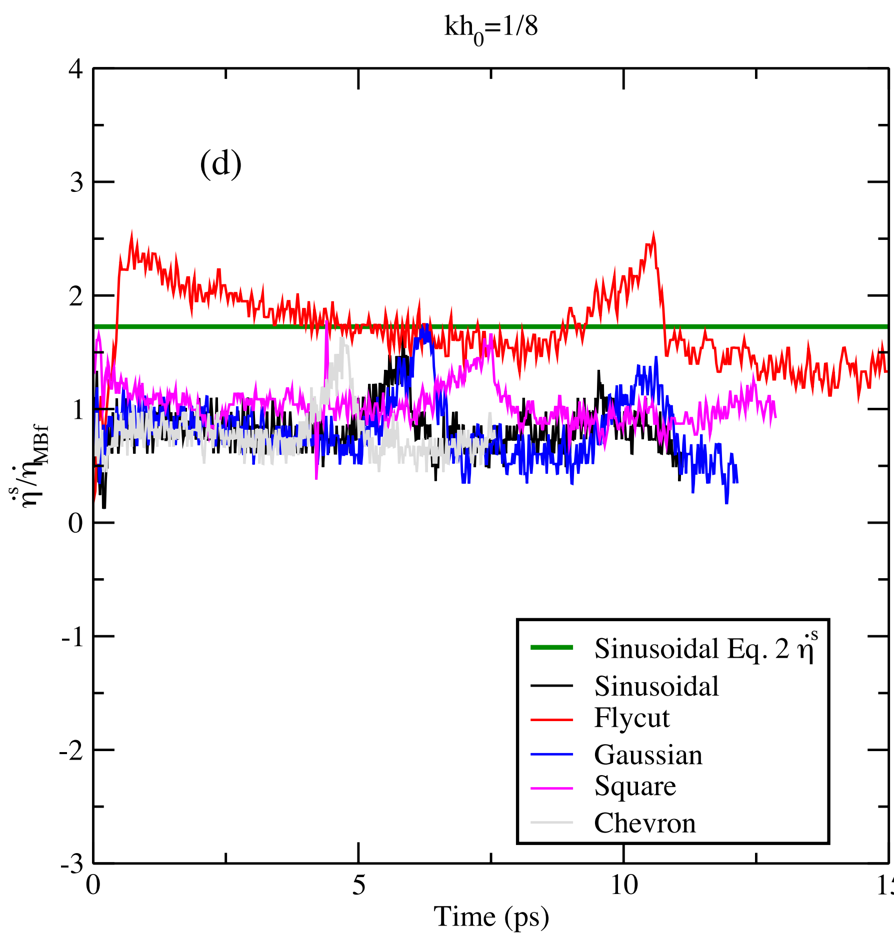


Spike heights and velocities for kh_0=1.0

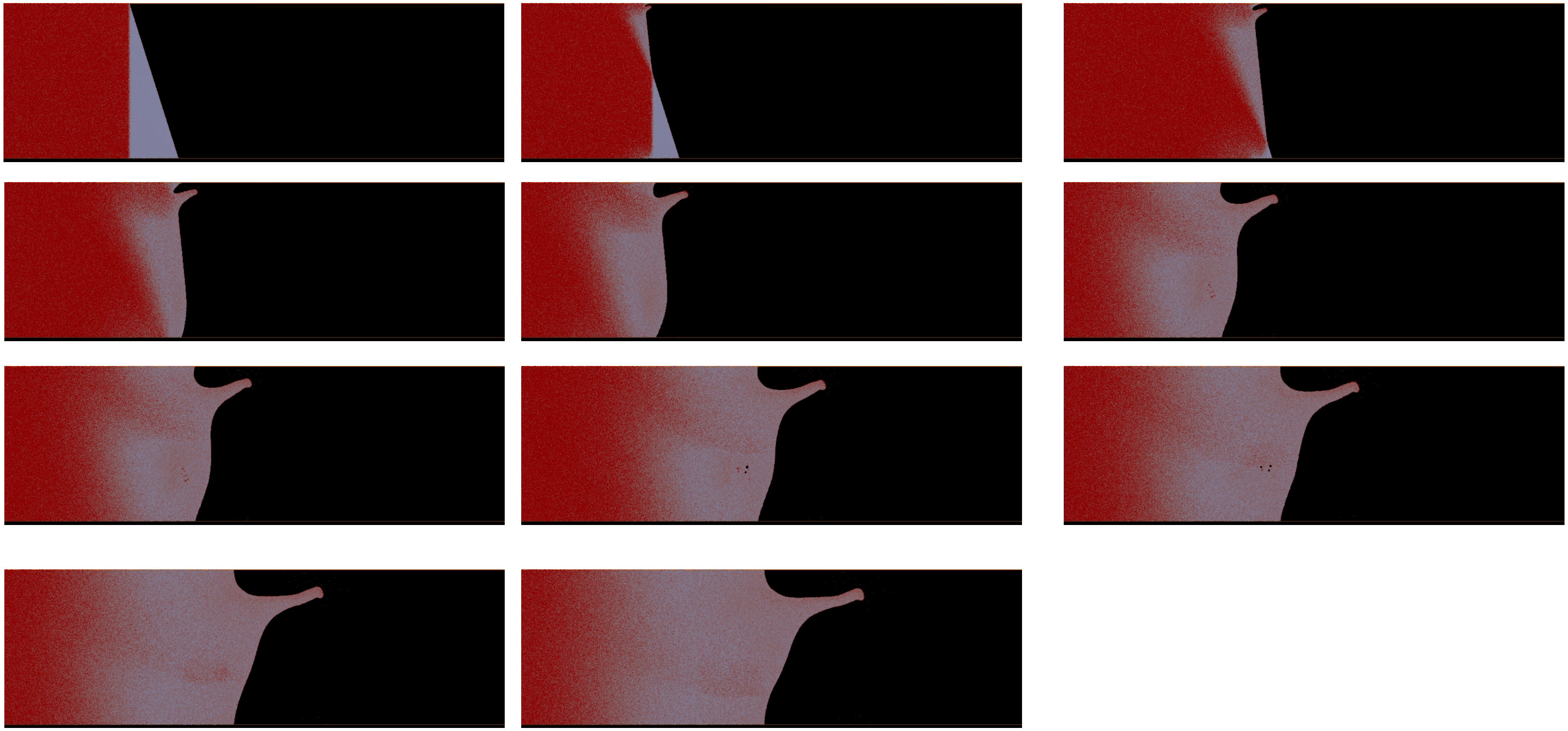


Spike heights and velocities for kh_0=0.125

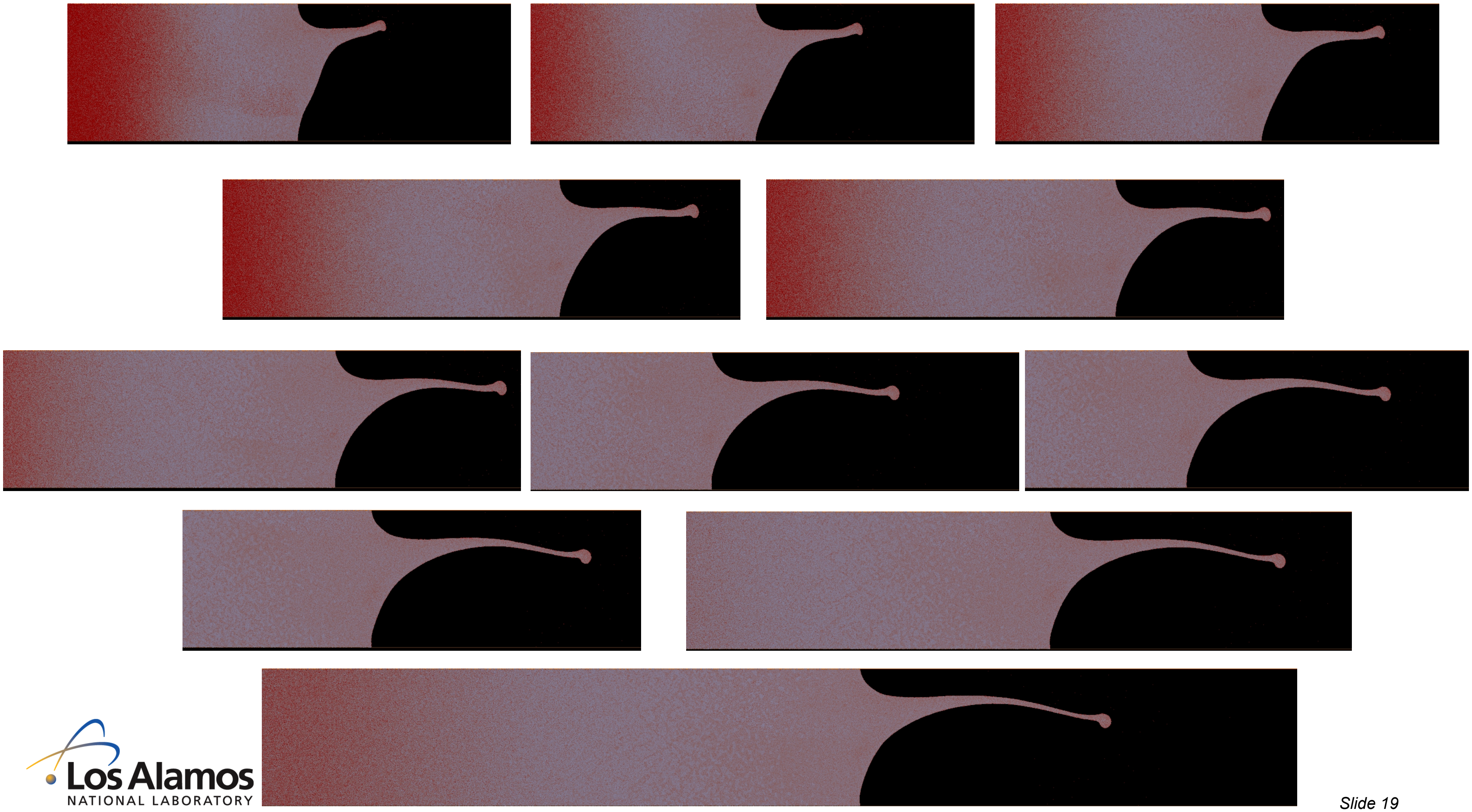




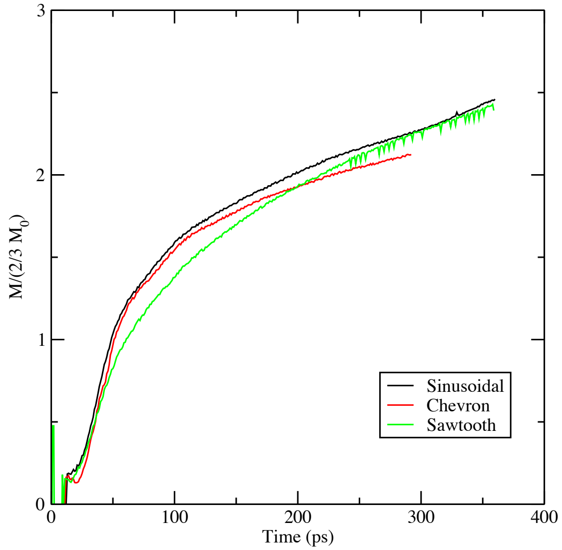
Images from Sawtooth from t=0-50 ps at 5 ps intervals



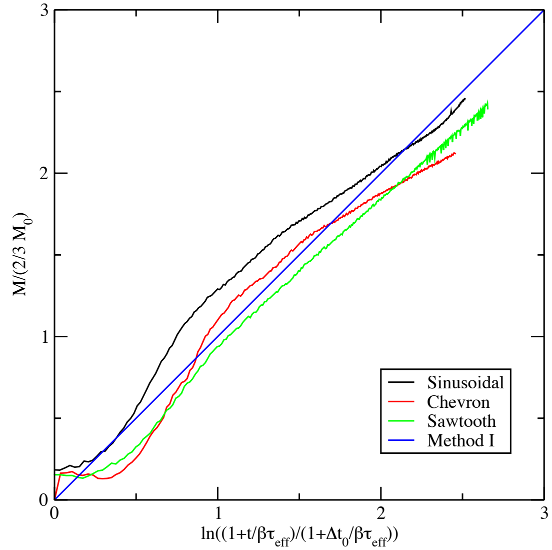
Images from Sawtooth from t=50-150 ps at 10 ps intervals



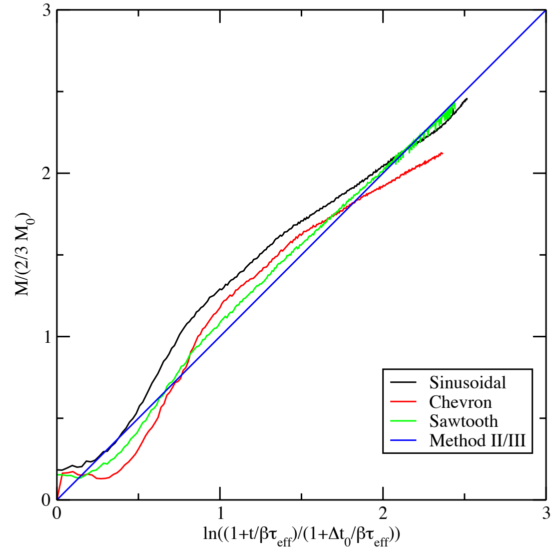
Mass from sinusoidal, chevron, and sawtooth kh_0=1.0



scaled mass vs time

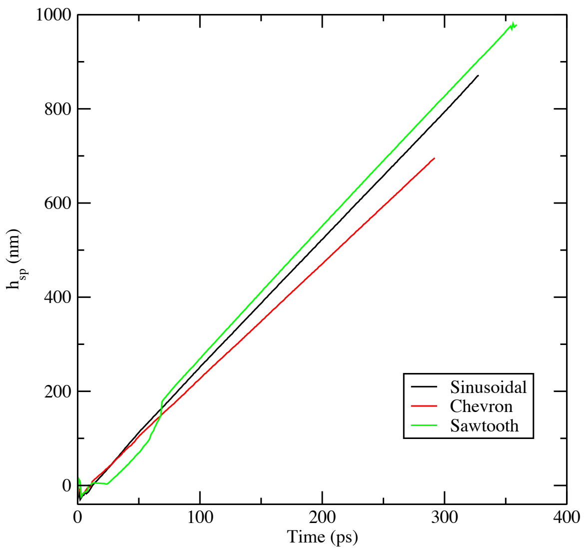


Method I--kh_0

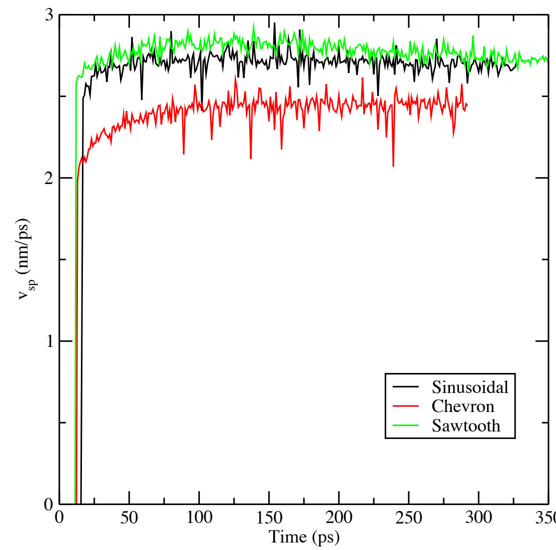


Method II or III--kh_{0f}

Spike heights and velocities



Spike Height



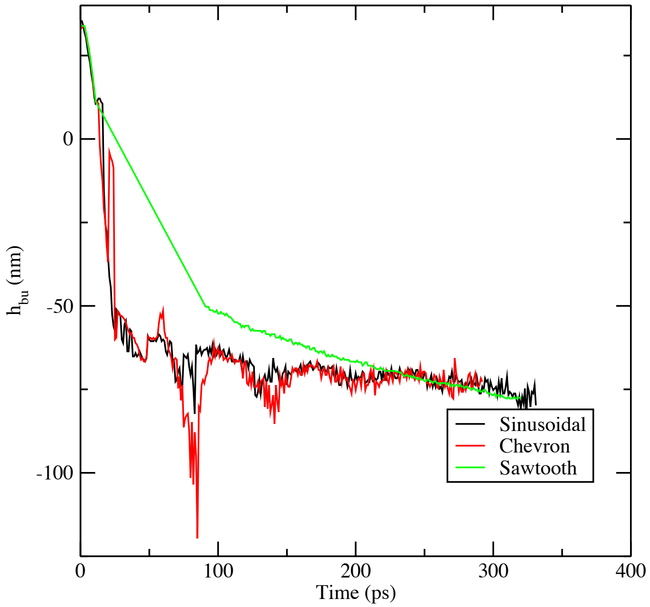
Spike Velocity

- **Spike height below 100 ps for the sawtooth shape is difficult to determine with the information that is coming out of the simulations due to the lack of symmetry about the middle of the simulation. It will also be observed in the bubble height and velocities shown on the next slide.**

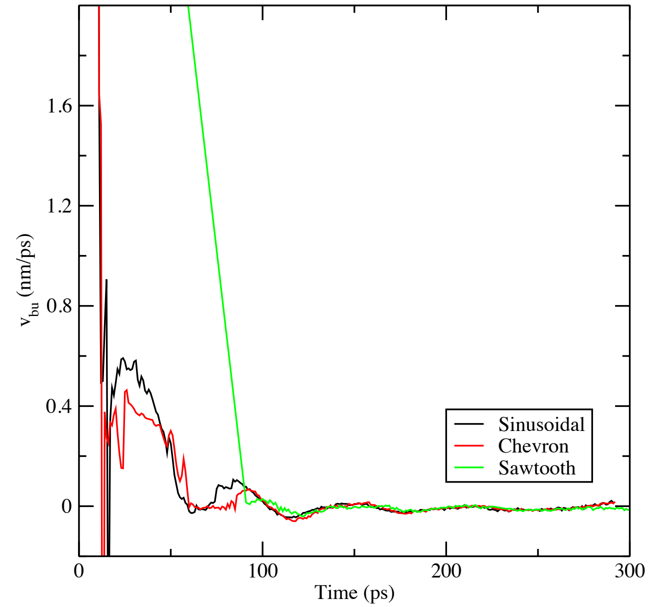
Bubble heights and velocities

- **Bubble heights for the sawtooth are complicated as per note for the spike position. Furthermore the bubble velocities are even harder to obtain and thus the bubble velocities below about 100 ps are not reliable.**

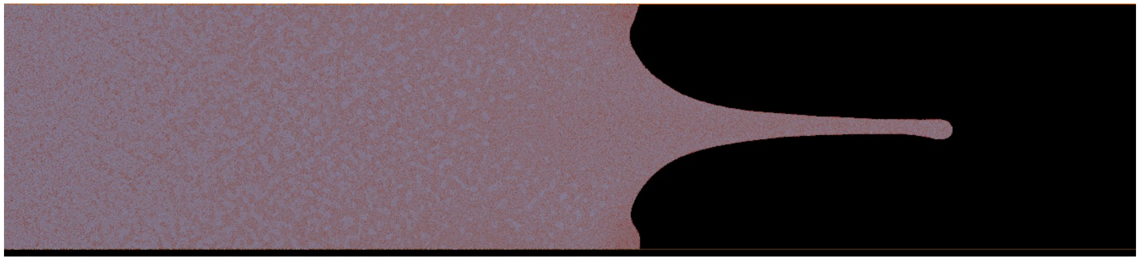
Bubble Height



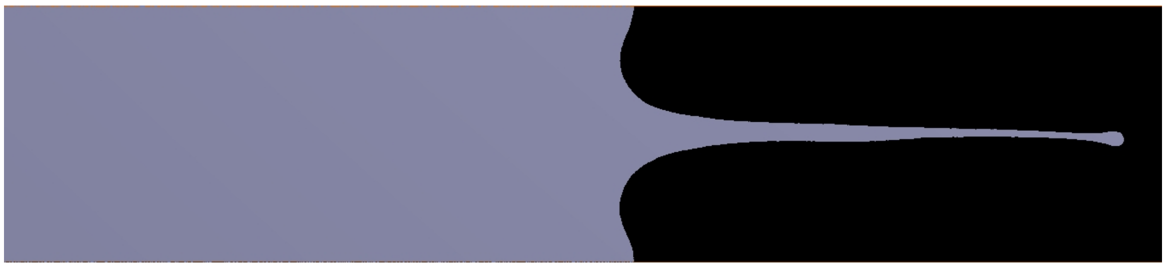
Bubble velocity



Preliminary comparison of copper MD simulations Sinusoidal/Flycut(aka Buttler scoops) at t=160 ps



- Sine v_{sp}= 1.829 nm/ps with an initial, v_{sp0} = 1.575 nm/ps

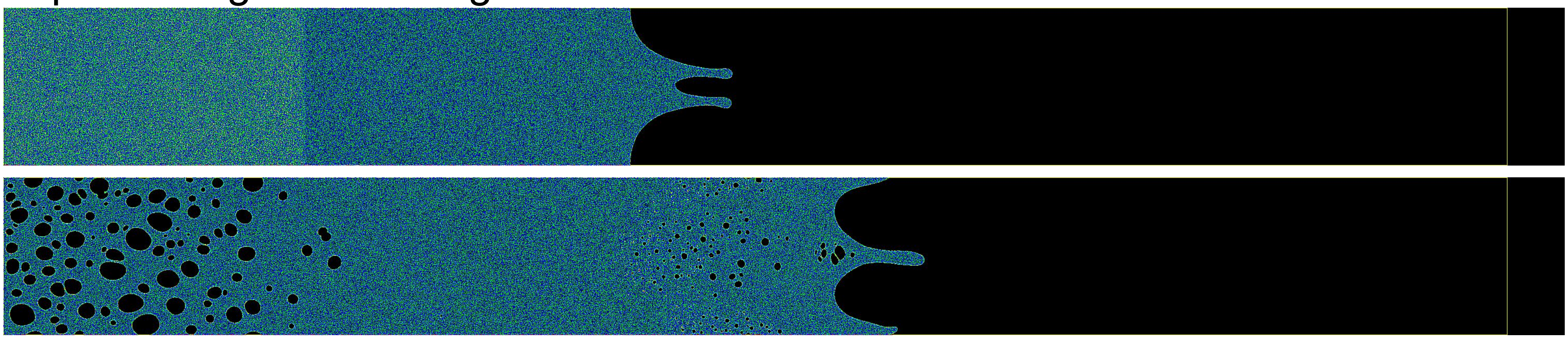


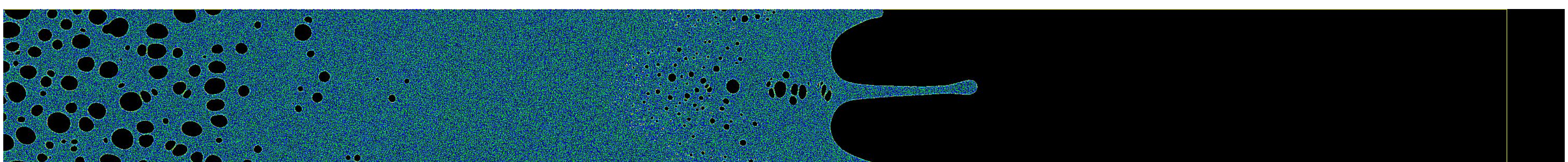
- Flycut(aka Buttler scoops) v_{sp}=2.951 nm/ps

$$\frac{V_{sp}^{Flycut}}{V_{sp}^{Sinusoidal}} = 1.613$$

Multimode simulations with double shocks

- Initial surface has 2 wavelengths with the same amplitude superimposed upon a single wavelength wave





- Same time as multimode above.

Conclusions and future work

- **The results for the collapse of the areal mass predicted by the model does a good job although there still needs some work on the analysis of the spike velocities.**
  - One approach will be to analyze more completely the simple two Fourier modes like just shown paying close attention to the velocity interaction.
- **The bubble velocities do show the behavior as predicted by the longest mode of the Fourier series.**
- **Initial reported literature behavior of ejecta breakup with molecular dynamics appears to be affected by small shock direction lengths and may show percolation of the defects into the bubble region.**