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Institutional Computing Annual Report 2014
Project: W13_sdtnanoc
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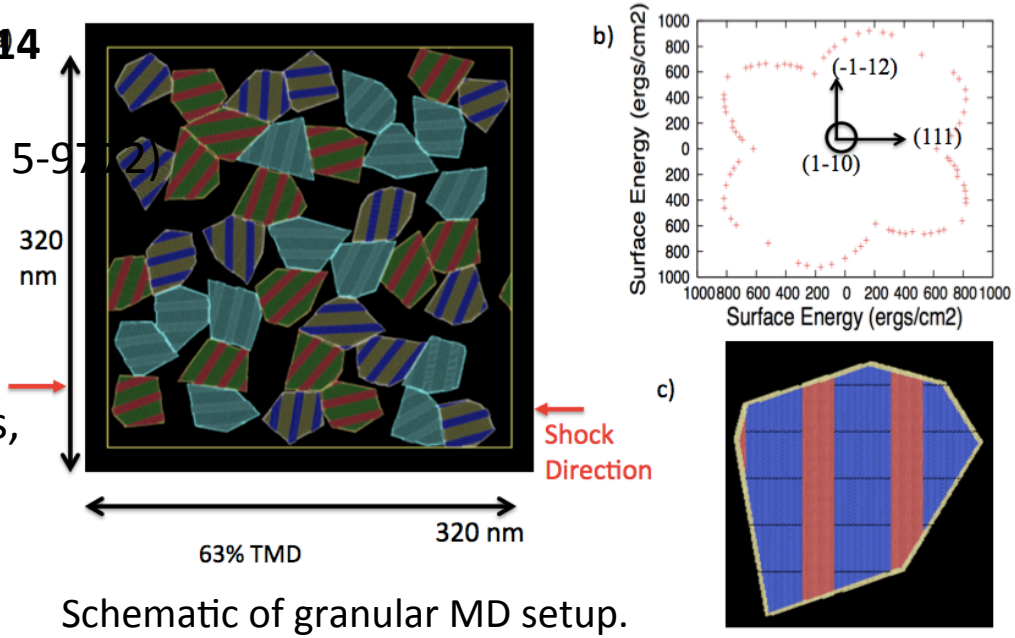
First fully atomistic simulation of a granular material.

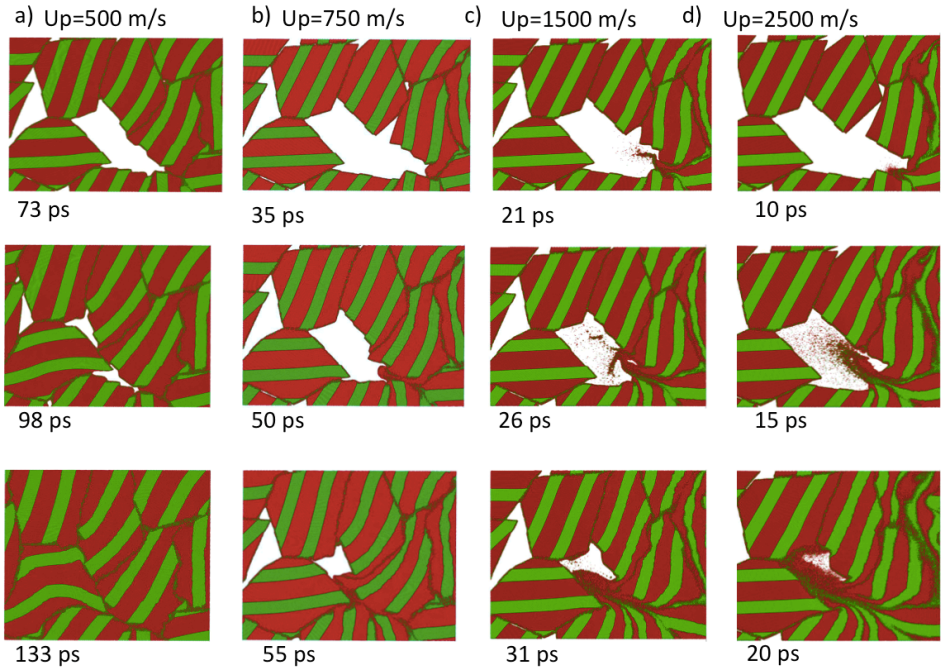
Grains built to prefer low energy faces.

Diffuse, broad shocks at low piston velocities, but, sharper shocks for stronger impacts.

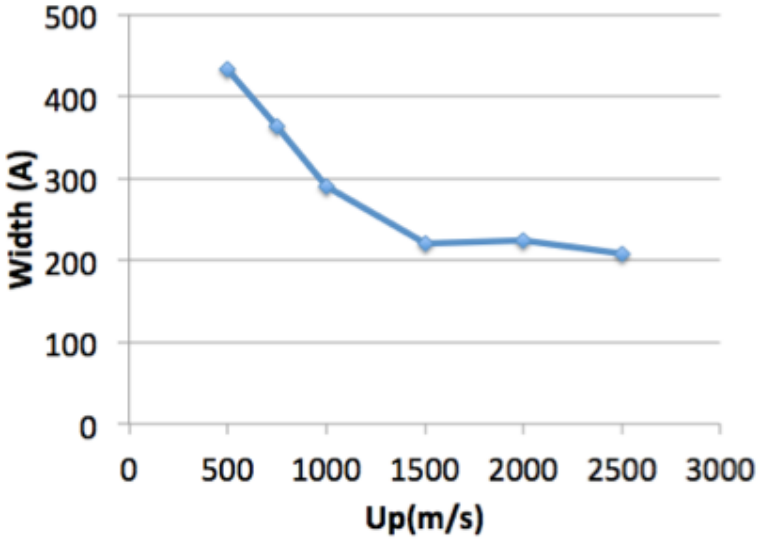
Consequence of change in nature of ejecta.



Schematic of granular MD setup.

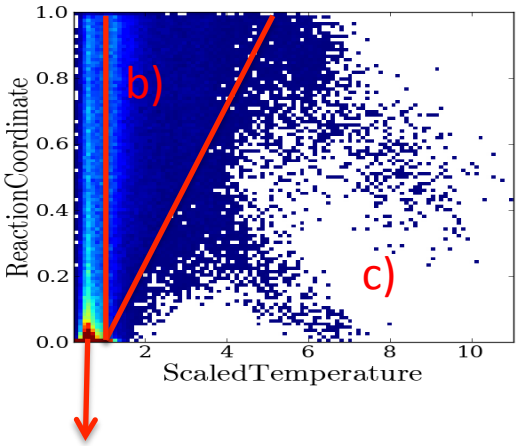


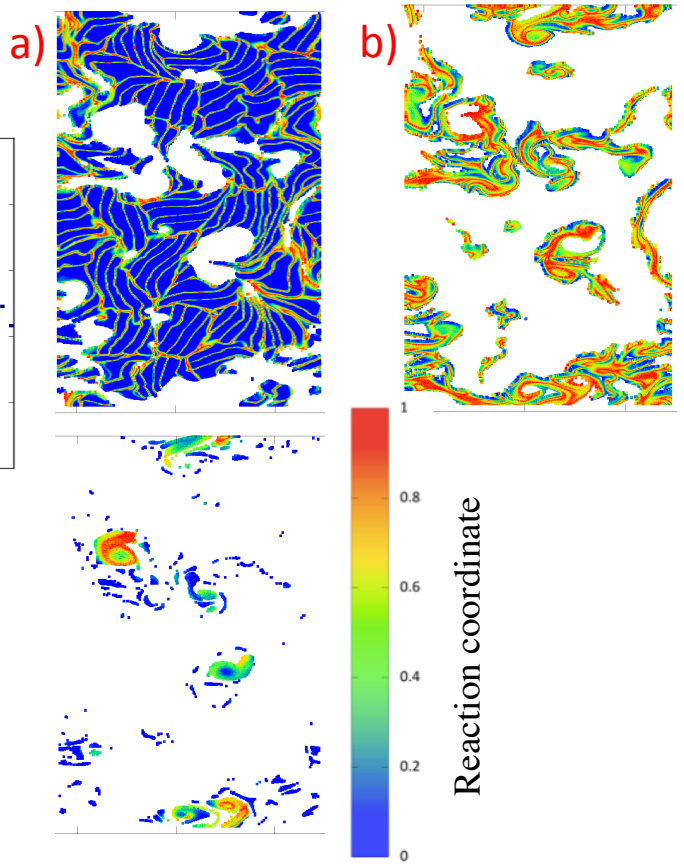
Transition in mechanism of void closure:
plastic deformation-> extrusion-> fluid jetting



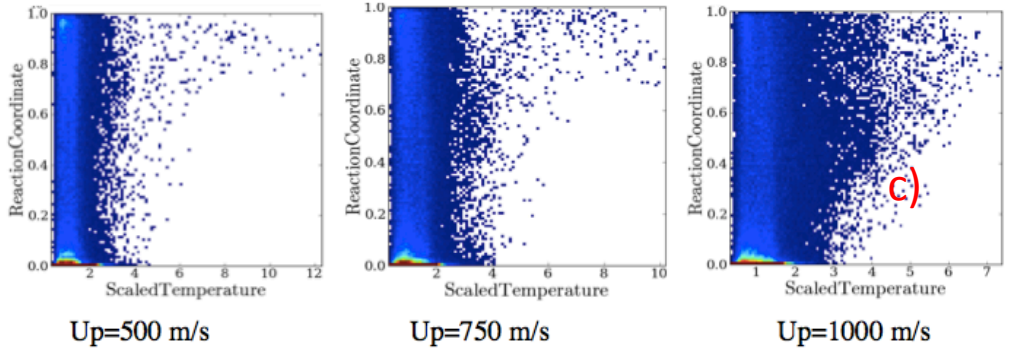
Width of the shock front as a function of piston velocity

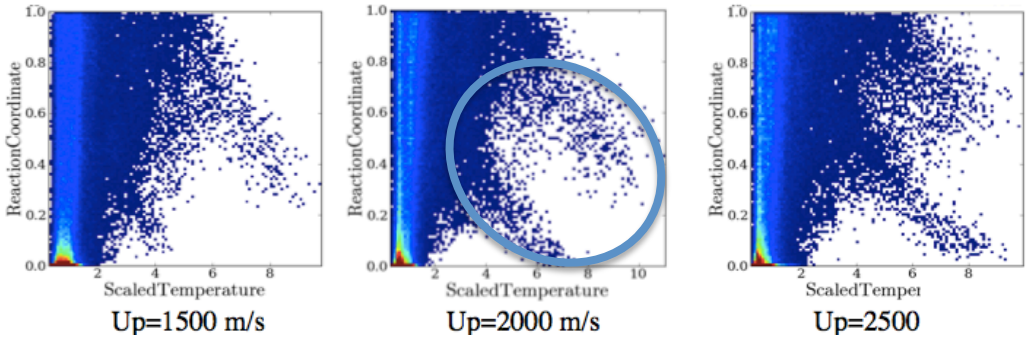
- Porosity not just hot-spots.
  - Sites of accelerated mixing.
  - Redirects shock energy to translational K.E.
  - Provide alternate reaction paths.
    - Convective mixing as opposed to diffusive in the bulk.
- Increased non-equilibrium at higher impact velocity.





Alternate reaction paths b) and c) provided by the porosity.





Correlation maps of reaction progress against temperature showing increased non-equilibrium effects at higher impacts.