Multi-material Athena++ with Mie-Grüneisen EOS

For Planetary Science and Shock Physics Applications

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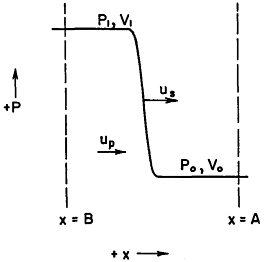
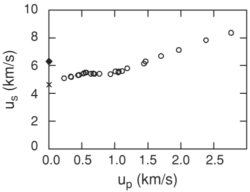
Domain of the fluid approximation

- Solids modeled as fluid in high pressure applications
- Pressures exceeds yield strength, material response
- Asteroid impacts: $\sim$ 15 km/s, $10^4 - 10^6 P_0$ (earth)



Rice et al., Solid State Physics (1958)

Shock experiments: Fe



Menikoff, *Empirical EOS for Solids* (2009)

MM-Athena++: Multi-material evolution model

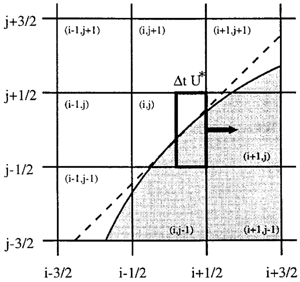
Material conservative equations coupled to basic hydrodynamic equations

$$\partial_t f_k + \partial_i(f_k v^i) = f_k \frac{\bar{\kappa}}{\kappa_k} \partial_i v^i$$
$$\partial_t \rho_k + \partial_i(\rho_k v^i) = 0$$

Mixed cell: pressure equilibrium

$$\bar{U} = \sum_k u_k(\rho_k, \bar{P})$$

u_k includes $\bar{P} d\mathcal{V}$ and shocks



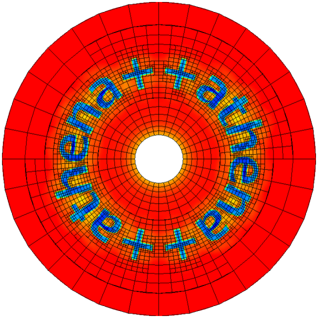
Miller & Puckett, Journal of Computational Physics (1996)

Cheng & Aslam, *In preparation* (2019)

Implementation into Athena++

Multi-material evolution with ideal gas / Mie-Grüneisen Murnaghan

- Book-keeping of data structures f_k, ρ_k, u_k
- Hydro evolution for f_k, ρ_k, u_k
  - Reconstruction
  - Riemann solver / Flux: sound/contact speeds
  - Source terms
- Equation of State
  - Book-keeping of parameters
  - Analytic EOS functions
  - Sound speeds (Bulk/Roe)
  - Mixed-cell closure models



Athena++: https://princetonuniversity.github.io/athena/

Cheng & Aslam, *In preparation* (2019)

Water/Granite: model vs experimental data

Hydro code: $P(\rho, e)$, $e(\rho, P)$

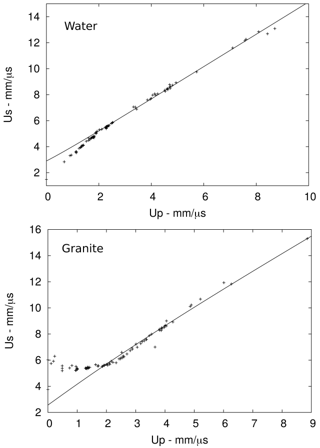
Mie-Grüneisen Murnaghan

$$P(\rho, e) = P_{\mathrm{ref}}(\rho) + (e - e_{\mathrm{ref}})\rho\Gamma(\rho)$$

P_{ref}, e_{ref}, Γ depend on κ_0, κ_0', Γ

Hugoniot fit: κ_0, κ_0', Γ

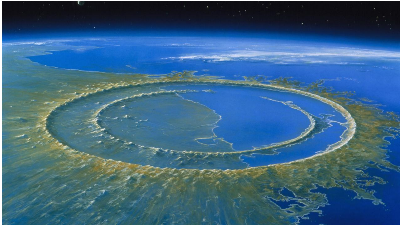
U_p: velocity behind shock
U_s: shock velocity

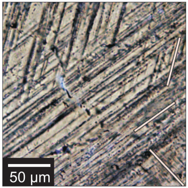


Cheng & Aslam, *In preparation* (2019)

Alvarez Hypothesis: large asteroid impact

- Evidence from sedimentary Cretaceous-Paleogene (K-Pg) boundary
- Concentration of iridium ($\times$100 normal), expected to be rare in Earth's crust
- Meteorites/asteroids contain high iridium concentrations
- Shocked quartz, indicative of a large impact event

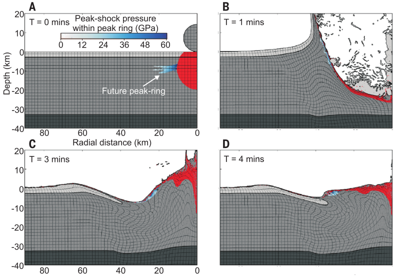




Morgan et al., Science (2016)

Dynamic collapse model

- Impact mixes near-surface rocks with deeper material
- Peak rings form from the collapse of central peaks



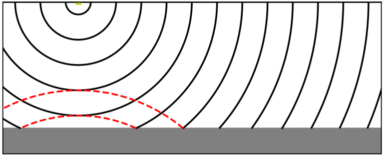
Morgan et al., Science (2016)

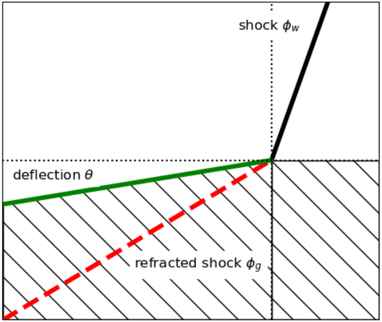
Numerical challenges in multi-physics for a wide range (3D) in lengthscale/timescale

- hydrodynamics (*km*)
- multi-material evolution
- material equation of state
- material strength models
- fracture models (μm)

Toy model for Chicxulub crater

Shock travels through water, transmitted through granite.

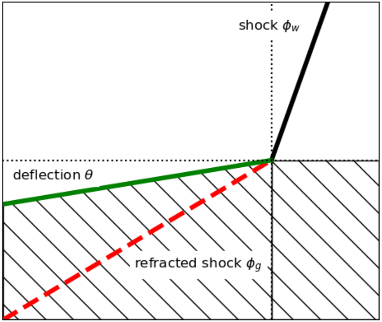




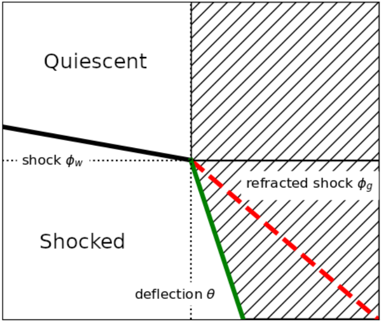
Cheng & Aslam, *In preparation* (2019)

Transformation to local interface frame

Toy model of interface



Local frame of shock interface



Cheng & Aslam, *In preparation* (2019)

Parameterize jump with shock polars

EOS $e(\rho, P)$

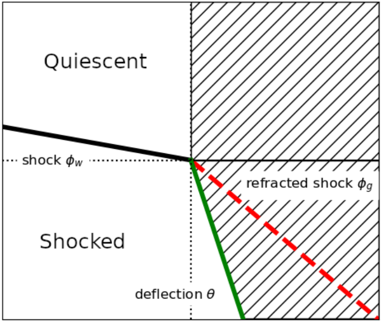
Hugoniot jump conditions

$$\rho/\rho_0 = U_s(U_s - U_p)^{-1}$$
$$P - P_0 = \rho_0 U_s U_p$$
$$e - e_0 = \frac{1}{2}(P + P_0)(\rho_0^{-1} - \rho^{-1})$$

Shock polars

$$\theta = \tan^{-1}\left[\frac{D_0 \sin\phi}{U_s - U_p}\right] - \phi$$
$$\phi = \cos^{-1}\left[\frac{U_s}{D_0}\right]$$

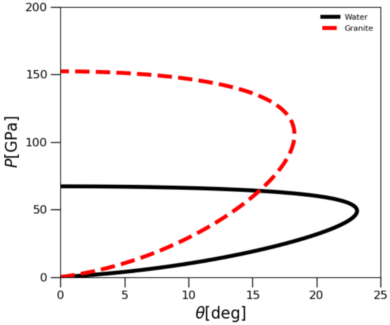
Local frame of shock interface



Cheng & Aslam, *In preparation* (2019)

Exact solution with shock polar analysis

Shock polars

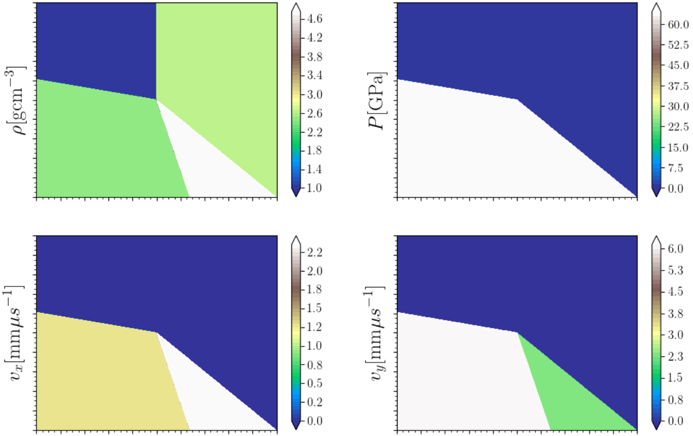


- 2D self-similar solution
- Direct comparison with numerical results
- Demonstrates robustness of mixed material model
  - Pressure equilibrium
  - Velocity slip at interface

Cheng & Aslam, *In preparation* (2019)

Toy problem as shock polar solution

Convenient units: **Pressure** GPa = 10^4 bar = 10^6 Ba, **Velocity** km s^{-1} = mm μs^{-1}

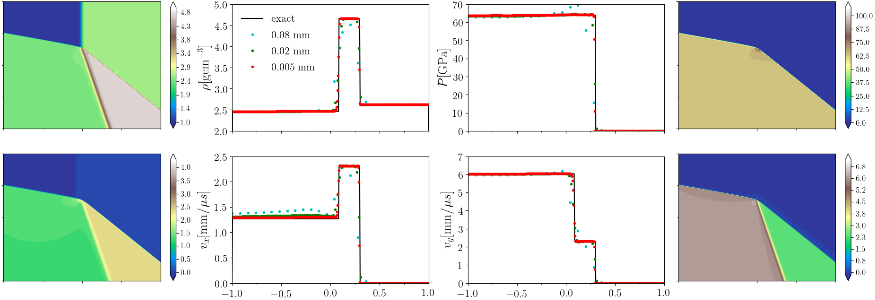


Cheng & Aslam, *In preparation* (2019)

Comparing simulation with shock polar solution

Method: rk3 / recon2 / LLF or HLLC

Consider (y_0, x), $t = 0.5\mu s$



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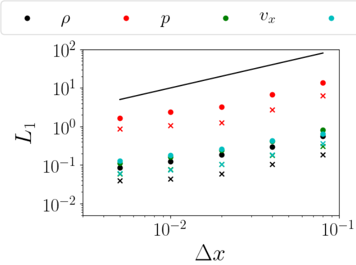
Sub-linear convergence: LLF (•) vs HLLC (×)



$$||E||_1 = \Delta x \sum_i^N |E_i|$$

- Results less than 1st order in presence of shocks
- Spurious high pressure regions due to mixture model
  - Errors with f_k
  - Problems with slip
- Improvements needed
  - Interface tracking method
  - Multi-phase velocities

Cheng & Aslam, *In preparation* (2019)

Summary and future work

New MM-Athena++ multi-material hydrodynamics code soon-to-be available for planetary science applications

- Evolution of multiple materials obeying separate equation of state
- Assumes pressure/velocity equilibrium for mixed cells
- Ideal gas and Mie-Grüneisen Murnaghan equation of state

Future development

- Multi-phase velocities: different for each material
- Equation of state: new analytic models, tabular form
- Strength/fracture models
- Reacting flows for high explosives applications