High-Speed Reactive Flow

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Scope of present discussion:

Mathematical models and computation of detonation in heterogeneous (solid) explosives.
(see MS3 and MS7, for example, for issues related to DDT in homogeneous explosives)

General issues:

- Complex microstructure (see micrograph).
- Difficult thermo-mechanical response to initiating stimulus (hot spot formation).
- Incomplete equation of state and reaction rate information.
- Description involves multiple physics, multiple scales and multiple phases.

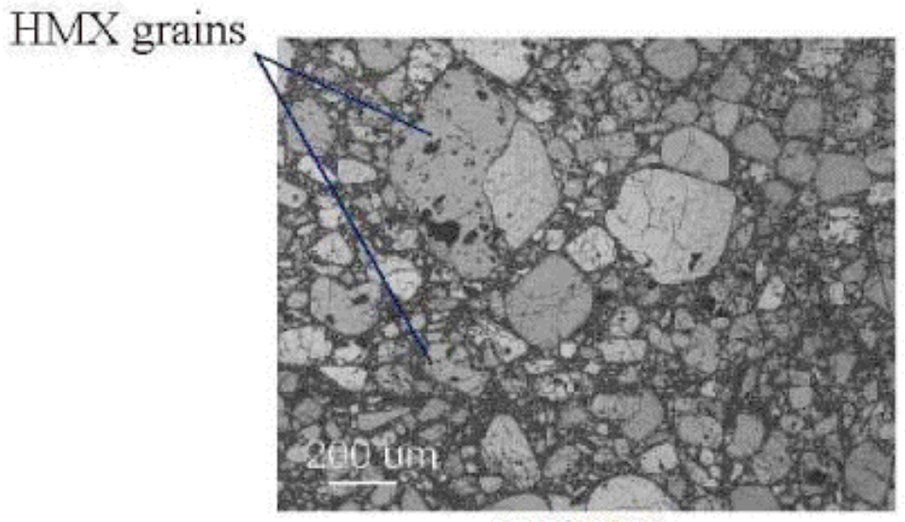

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Photo courtesy of Dave Phillips and Cary Skidmore

Modeling Issues

- Current macro-scale models:
  1. Homogeneous mixture models, e.g. ignition-and-growth
  2. Multiphase models, e.g. two-phase Baer-Nunziato

- Challenges (macro-scale models):
  - Uncertainty in the constituent equations of state for both models (1) and (2).
  - Construct accurate mixture EOS for (1).
  - Develop suitable reaction rate models for both (1) and (2).
  - Coupling of (1) and (2) to a model for an inert to handle compliant confinement.

- Challenges (micro-scale coupling):
  - Multi-physics model required to study interaction of shocks in elastic-plastic solid with single or multiple gas voids.
  - Develop suitable models to study the effect of grain-scale morphology on the development and growth of hot spots.
  - Develop suitable multi-scale model which couples micro-scale and macro-scale thermo-mechanical behavior.

Computational Issues

- Current methods for macro-scale models:
  1. Often based on shock-capturing for hyperbolic conservation laws.
  2. Include ODE solver for stiff source terms.
  3. Employ adaptive mesh refinement (AMR) to handle rapid spatial and temporal scales.
  4. Numerical approach to handle complex (perhaps moving) geometry.
  5. Parallel processing for large-scale runs (100M grid points or more).

- Challenges (numerical treatment of macro-scale models):
  - Accurate shock-capturing methods for reactive flow models with general equations of state (pressure reconstruction from cell-averaged values).
  - Develop high-order methods for multi-material reactive flow (reactive flow with interfaces between materials).
  - Develop methods for coupled multi-material and multi-phase models.

- Challenges (general):
  - Develop strong scalable AMR-parallel methods for large parallel machines (100K processors with multiple CPU cores: MPI-OpenMP model)
  - Develop methods for multi-domain, multi-scale, multi-physics models.