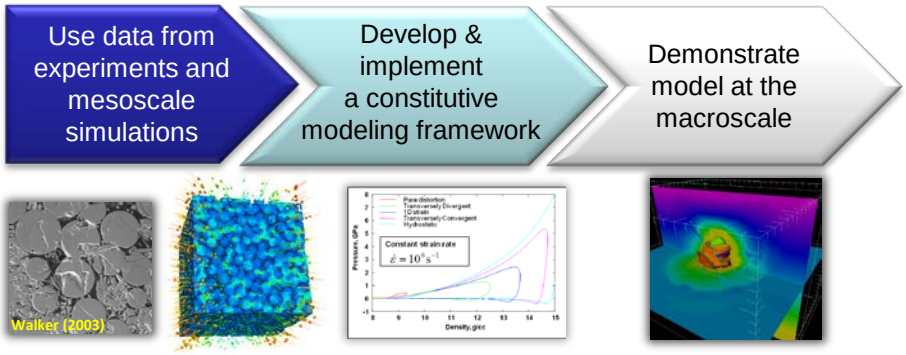
Mesoscale Priority Research Direction

Application of Mesoscale Simulations Toward the Development of Predictive Models for Deformation and Failure of Heterogeneous Granular Materials

Opportunity

"Materials by design" for extreme dynamic environment applications has been a long-standing goal of the scientific community. Enabling this new paradigm requires predictive models that can relate the dynamic response of the material to physical and microstructural properties. Mesoscale simulations, validated with experiments at appropriate scales, can be a powerful approach that can help with the development of these predictive models.

Approach



Code improvements, and novel experiments and diagnostics are needed to enable physically realistic mesoscale simulations

Meso Challenge

- **How does the microstructure evolve at the mesoscale?**
- **Are properties of the porosity beyond void fraction important?**
- **How can the effect of inter-particle friction be determined?**
- **What role does fracture play in the evolution of the particles?**
- **How can a macroscale model be formulated to include the complex mesoscale behavior?**

Answering these mesoscale questions provides important clues about the macroscopic response of heterogeneous granular materials, paving the way for the development of physically motivated predictive models for material behavior at the continuum level.

Impact

Predictive models that relate deformation and failure of heterogeneous granular materials to physical characteristics like morphology and particle size distribution will enable simulations with unprecedented details, paving the way for a new paradigm of materials by design whereby the microstructure of the material can be optimized to withstand the rigors of specific extreme environment applications. Discoveries made during this effort will provide a fundamental understanding of heterogeneous material response with implications for a wide range of DOE missions including both energy and national security applications.

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