



U.S. ARMY  
**RDECOM**

Multiscale Reactive Modeling for Energetics

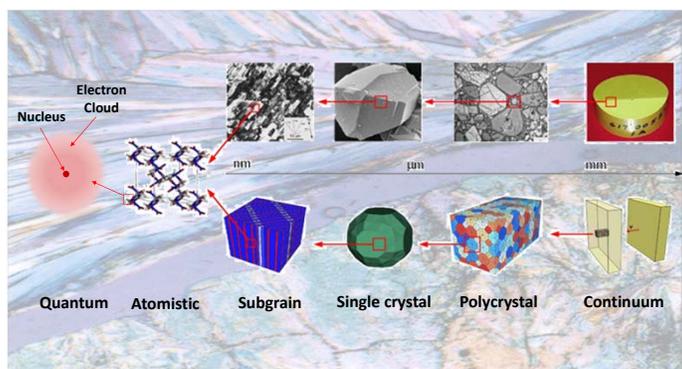


**S&T Campaign: Sciences for Lethality & Protection**  
*Ballistics and Blast*

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**Research Objective**

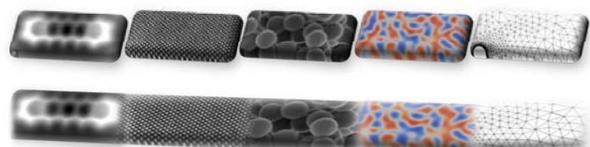
- Develop a validated, science-based multiscale modeling and simulation capability to simulate energetic material (EMs) response to insults
- Validated quantum-informed models that capture the effects that reactions and microstructural heterogeneities impose on macroscopic events



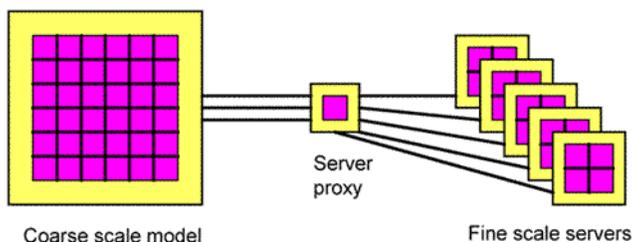
Modeling EM response involves the full range of material scales

**Challenges**

- Multiphysics and multiscale coupling
- Verification/Validation, Uncertainty Quantification
- Theoretical, experimental methods for relevant length scales, multiscale theories



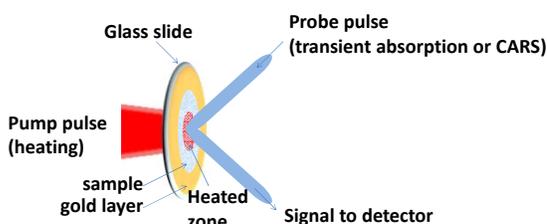
“apparent” seamless integration across length scales as needed



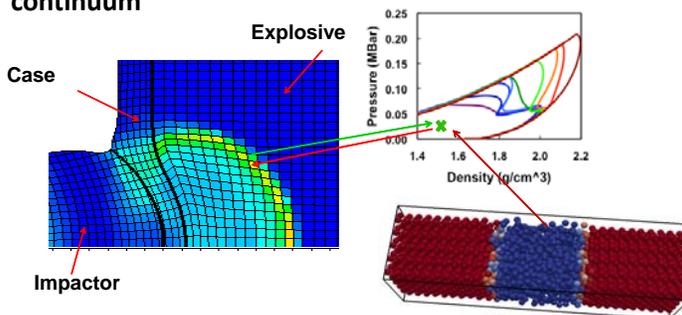
Predictive, lower-length scale simulations to provide the material response in large-scale continuum simulations

**ARL Facilities and Capabilities Available to Support Collaborative Research**

- Ultrafast pump-probe diagnostics of material response to shock, optical excitation or thermal insult
- Ultrafast indirect flash heating of thin film energetic materials and polymers



- Laser photoacoustic and force-distance spectroscopy of energetic materials and polymers
- Access to supercomputers and storage systems at five DoD Supercomputing Resource Centers
- Specialized modeling/simulation tools to explore reactive response of EMs at scales ranging from quantum to continuum



- Process to directly use sub-grain simulation results in continuum simulations, replacing (empirical) material EOS.

**Complementary Expertise/ Facilities/ Capabilities Sought in Collaboration**

- Crystal growth and sample preparation for studying selected crystallographic faces.
- Laser shock facility with in situ diagnostics
- Mathematical methodologies for scale bridging
- Coherent high harmonic generation to study dynamics of an energetic crystal under stimuli
- Large scale coarse grain polycrystalline simulations of sintering / grain-growth / phase change during shock
- Suggestions for innovative new research approaches to address research challenges