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OVERVIEW OF ASC PEM & BRIDGING SCALES IN MATERIAL MODELING

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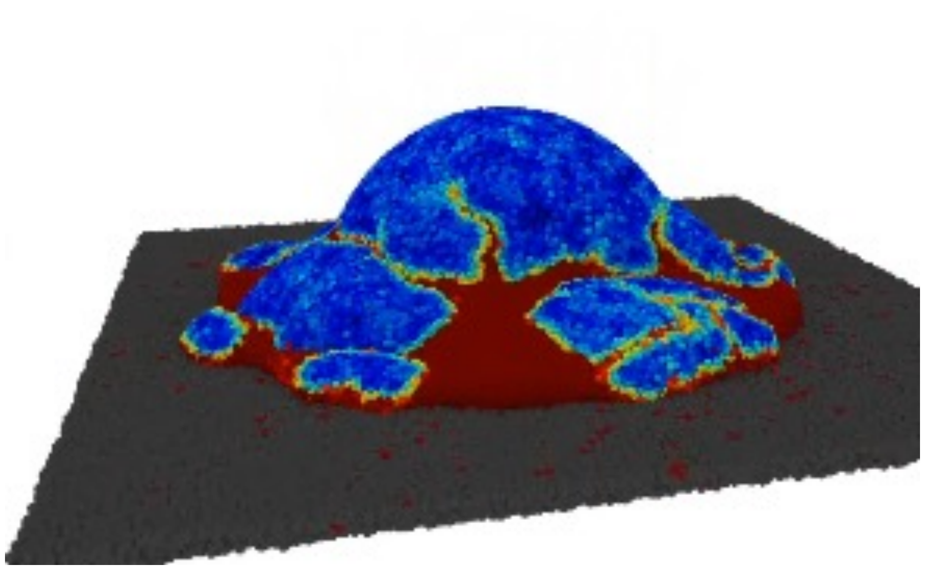
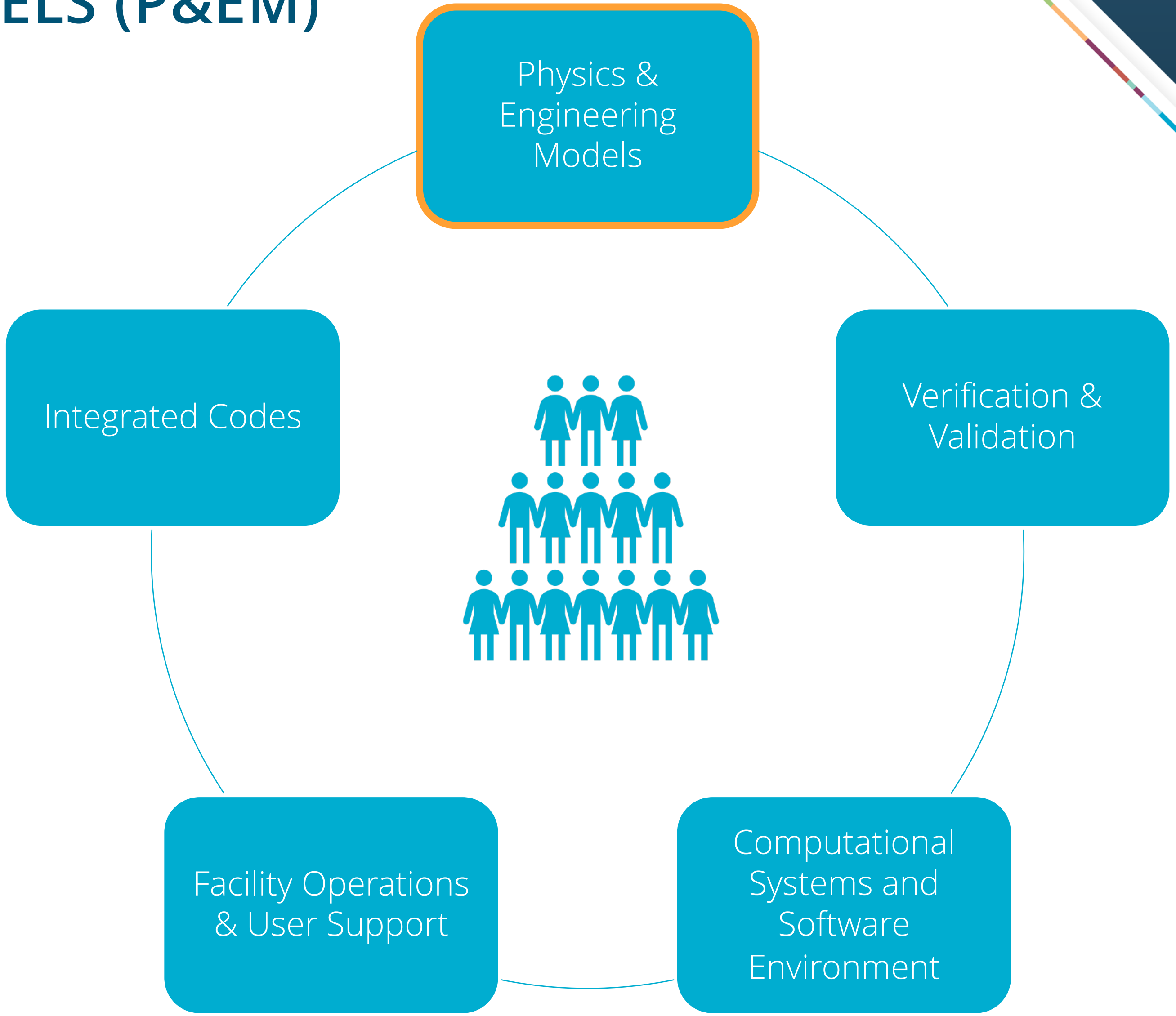
ASC PHYSICS & ENGINEERING MODELS (P&EM)

Physics & Engineering Models

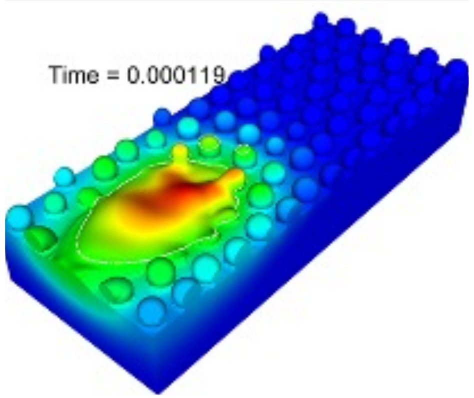
Provides science-based models, integrating theory, computational simulation, and experimental data to be used in simulations enabling design, production, qualification, surveillance, and assessment of systems & components.





ASC PHYSICS & ENGINEERING MODELS (P&EM)

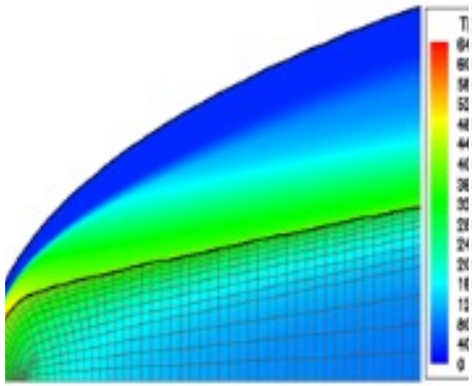
Production Processes



Optimize properties including residual stress state and variability.

Examples: weld modeling, additive manufacturing, foam encapsulation, thin-films & coatings, multi-phase

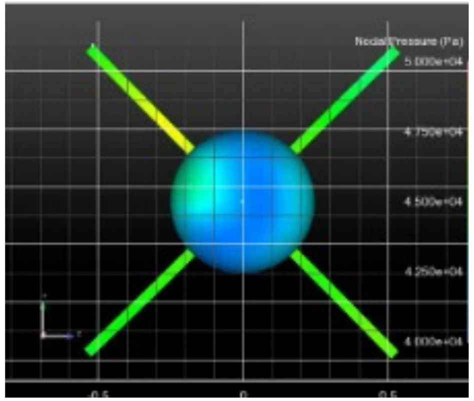
Environmental Loads



Combined environments for safety, performance, and survivability.

Examples: hostile encounters, delivery scenarios, accident environments, electromagnetics

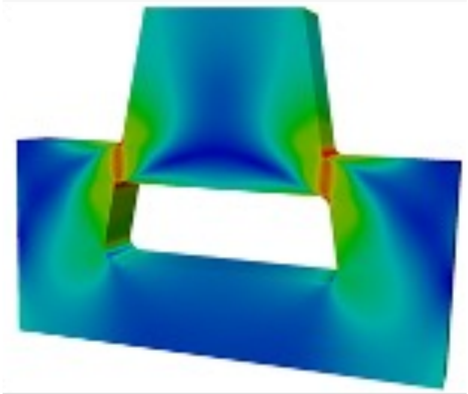
System and Component Response



Predicting performance in real environments.

Examples: stochastic pressure loading, environment specifications, system and component performance

Material Science and Mechanics



Material models for extreme loading conditions.

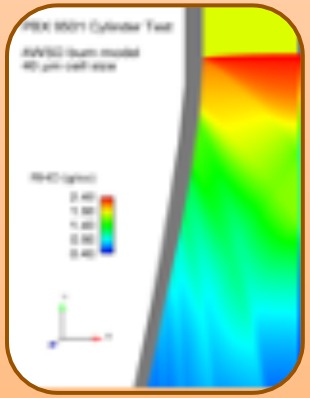
Examples: failure & fracture, EOS, thermal contact, particle scale dynamics, energetic material structure

EXAMPLES OF DISCIPLINES OF INTEREST TO NNSA FOR PSAAP IV

- Hydrodynamics
- **Turbulence**
- **Particle & Radiation Transport**
- **Atomic Physics**
- **Reactive & Energetic Materials**
- Chemical transformations
- Combustion
- Solid-solid phase transitions
- Plastic Flow
- Shock-assisted and shock-induced reactions
- Magnetohydrodynamics
- **Equations of state and constitutive properties**
- **Material damage and failure**
- Material stability
- Novel materials
- Nuclear properties and data
- Design of experiments for validation, including surrogate materials and environments
- **Engineering mechanics and design**
- **Molecular dynamics**
- **Electromagnetic effects**

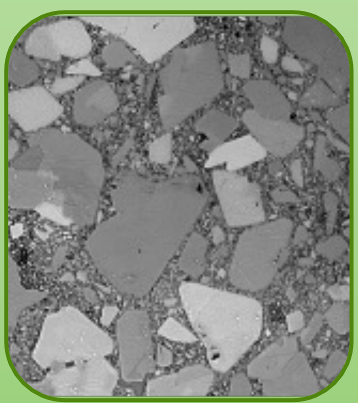
BRIDGING SCALES IN MATERIAL MODELING

Full-scale simulations



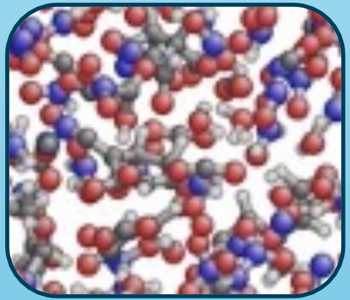
- Engineering & Physics Codes
- Performance
- Safety
- Model based

Meso-scale



- Large aggregate
- Realistic voids
- Model based
- Particle dynamics & mech.
- Material heterogeneity

Atomic-scale

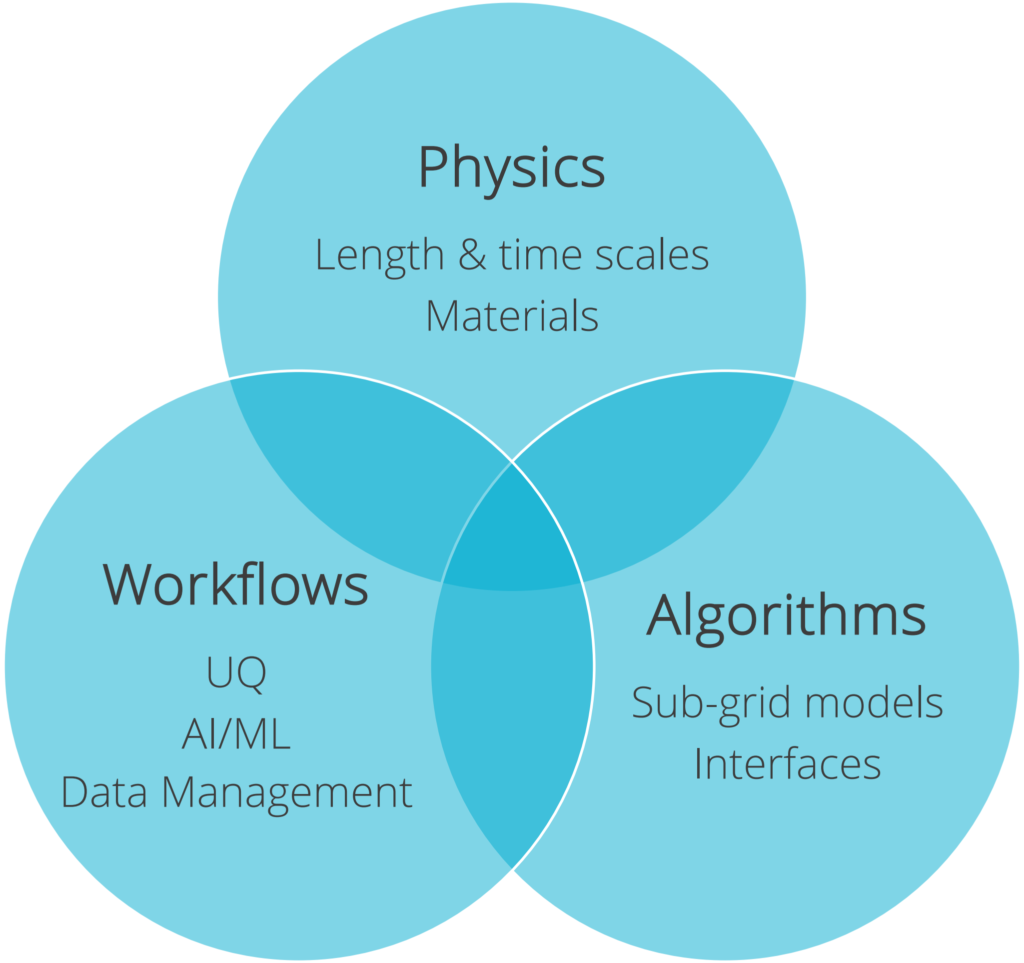


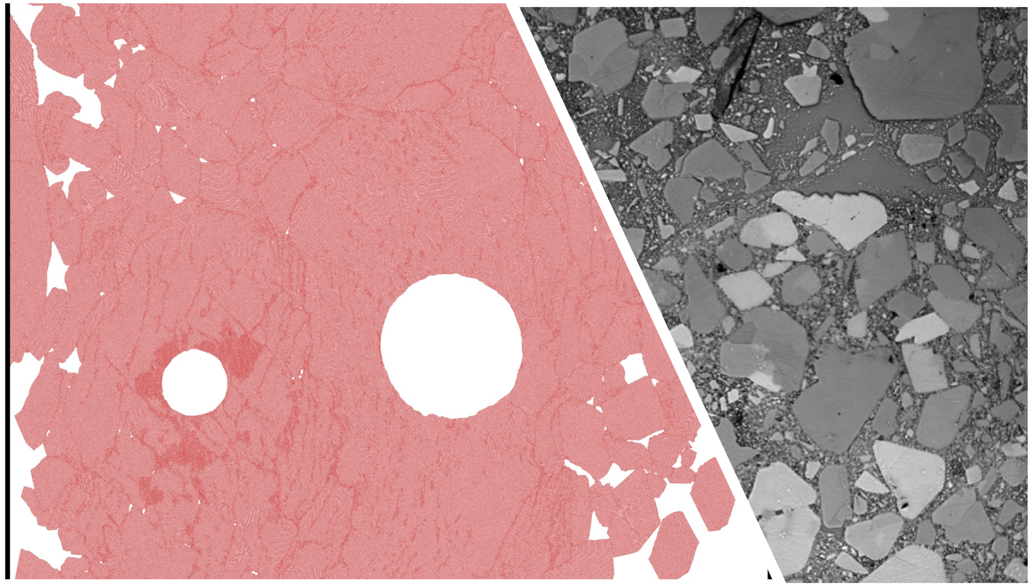
- Molecular Dynamics
- Single crystal
- Small aggregates
- Voids
- Deflagration studies

1nm | 100nm | 1um | 100um | 1mm | 1cm

BRIDGING SCALES IN MATERIAL MODELING

Advancements in exascale computing platforms, data science, software, and AI have made conditions ripe for successful investment in scientific and computing resources developing predictive modeling capabilities to bridge scales in material modeling.





BRIDGING SCALES IN ENERGETIC MATERIALS

Model energetic materials from manufacturing to performance and safety

The complexity and disorder in energetic material structure is key to understanding performance.

- The specifics of structure relate to feedstock characteristics, powder or paste formulation, processing, as well as component manufacture
- Component design, production, and qualification requires linking microstructure to performance in normal and off normal situations.

Meso-scale shock, thermal, electrical, ignition

Poly-crystalline thermo-mechanics

Energy localization at defects: void collapse, grain boundaries, interfaces, dislocation dynamics

Non-equilibrium molecular dynamics of flexible molecular crystals

BRIDGING SCALES FOR THIN-FILMS & COATINGS

Full-scale simulation of printing multi-layer devices is complex and must include thin-film coatings and other coating processes that span wide length scales.

- Macro-scale processing and printing
- Thin-film coatings: molecular, micro-, and meso-structure/behavior
- Other coating processes including solution deposition and growth
  - Physical Vapor Deposition (PVD) & Chemical Vapor Deposition (CVD)
  - Atomic Layer Deposition (ALD)

Synthesis
- Morphology
- Defects

→

Functionalization
- Structure
- Stability
- Aggregation

→

Layer Formation
- 3D-morphology
- Grain boundaries

→

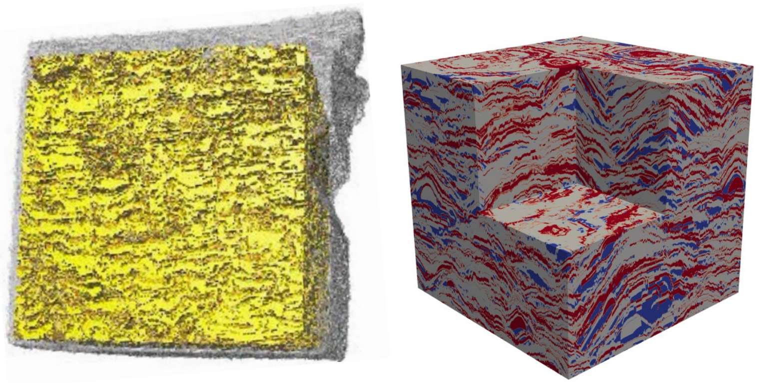
Multi-layer Devices
- Layers
- Interfaces
- Processing

BRIDGING SCALES FOR STOCHASTIC MATERIALS

Challenges in modeling radiation transport through stochastic media:

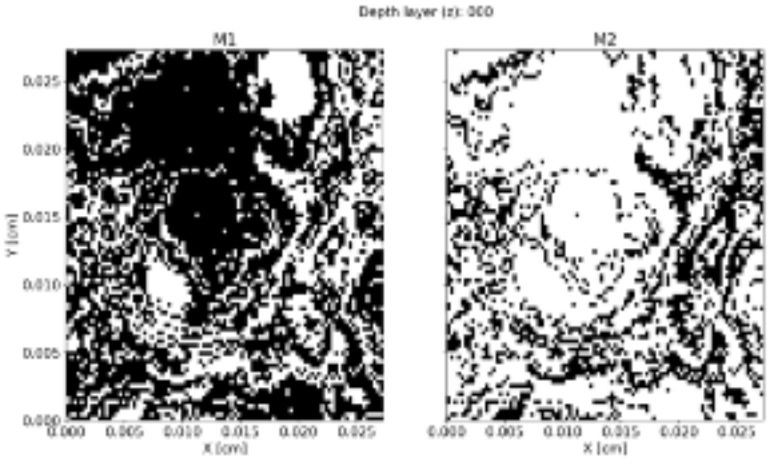
- Random structure is difficult to accurately and efficient model
- Random structure causes output uncertainties that must be quantified
- Many (expensive) calculations required for meaningful statistics

→ High computational costs

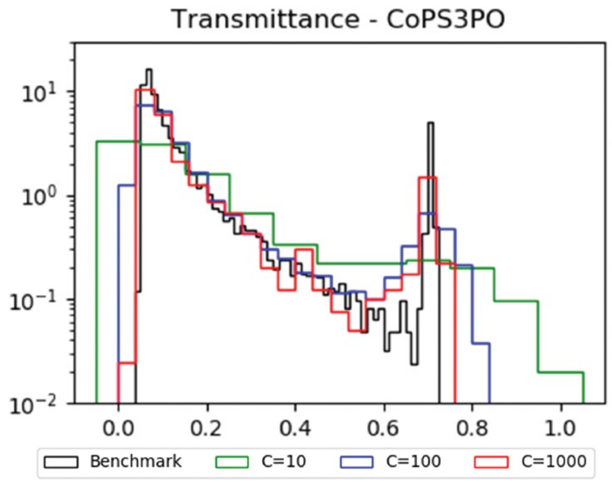


(Left) Experimentally imaged microstructures

(Right) Synthetically produced microstructures



Computed energy deposition in structure



Conditional Point Sampling (CoPS) computation PDF of transport outputs for various fidelity levels

THANK YOU