

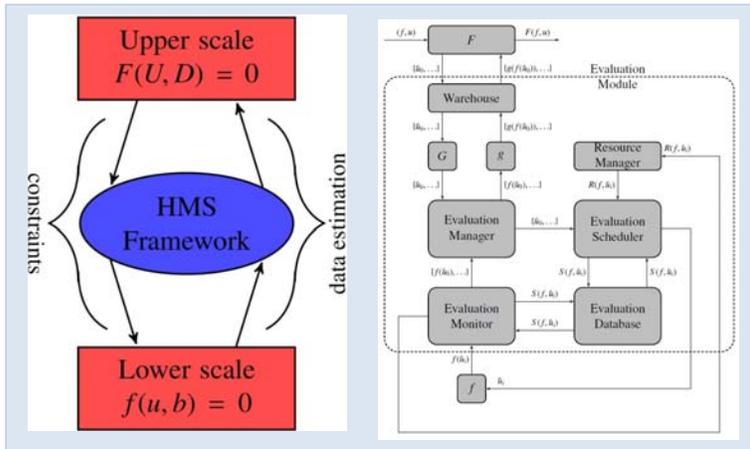


S&T Campaign: Computational Sciences
Predictive Simulation Sciences

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Research Objective

- Develop numerical and computational methodologies for scale-bridging in hierarchical (sequential and concurrent) multi-scale simulations of materials on extreme scale computing platforms



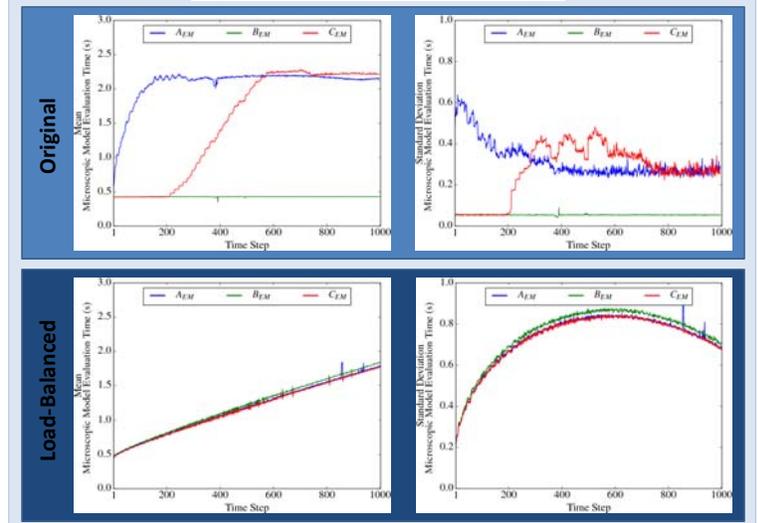
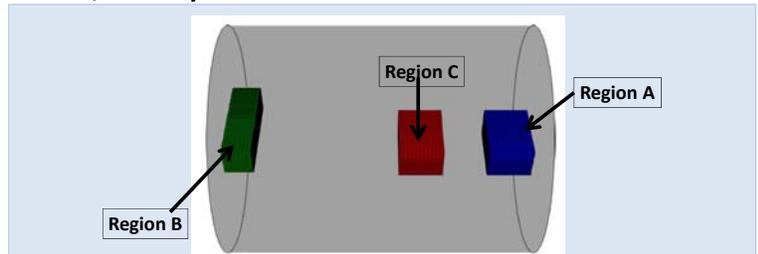
Two-scale hierarchical model.

Challenges

- Development of new multi-scale models is severely hindered by the lack of general numerical and computational methodologies for scale-bridging.
- Multi-scale material model hierarchy is usually adaptive and highly dynamic. However, current parallel computing environments remain static and lack support for adaption.

ARL Facilities and Capabilities Available to Support Collaborative Research

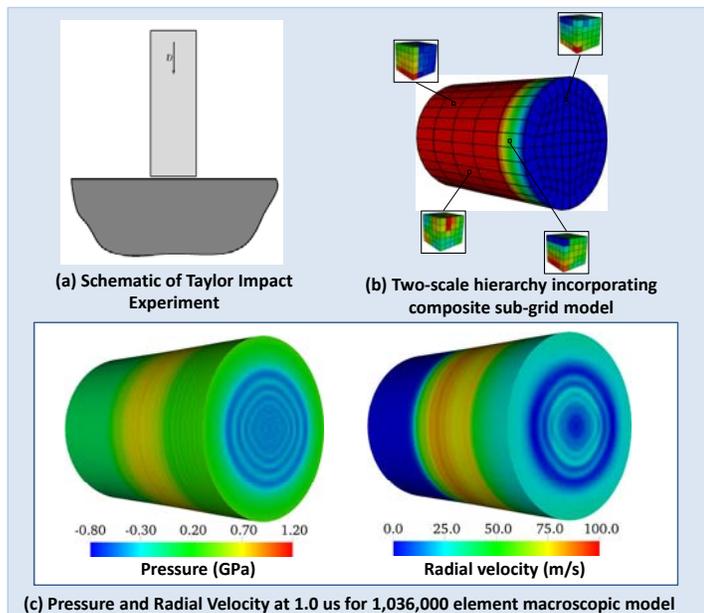
- Developed numerical methodologies, proof-of-concept implementation of scale-bridging framework and utilized it to construct multi-scale applications for electrochemistry and impact physics.
- Numerical techniques for adaptive generation of multi-fidelity surrogate-models under development.
- Publication describing scale-bridging framework submitted to International Journal of Numerical Methods in Engineering.
- Managing highly dynamic hierarchies, especially load-balancing and fault-tolerance, is critical to achieving practical multi-scale applications.
- Incorporation of surrogate models through methods such as adaptive sampling is necessary to alleviate computational cost, but may also exacerbate load imbalance.



Time evolution of the distribution of microscopic model evaluation times.

Complementary Expertise/ Facilities/ Capabilities Sought in Collaboration

- Methods for interpolation in high-dimensional spaces.
- Methods for interpolation on manifolds.
- Data estimation and analytics related to microscopic model response.
- Validation of our scale-bridging methodologies.
- Uncertainty quantification.



Taylor impact simulation of composite material.