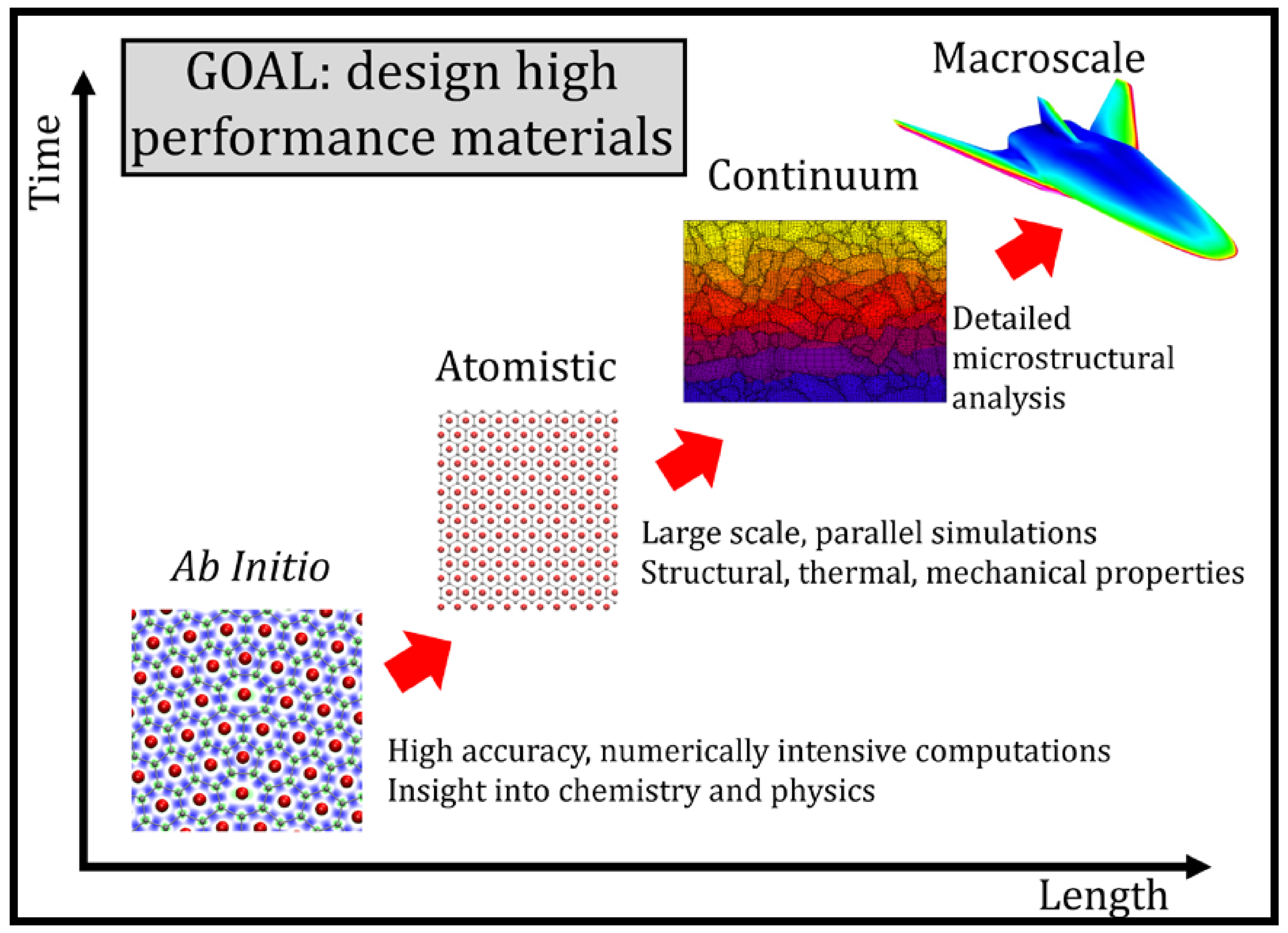
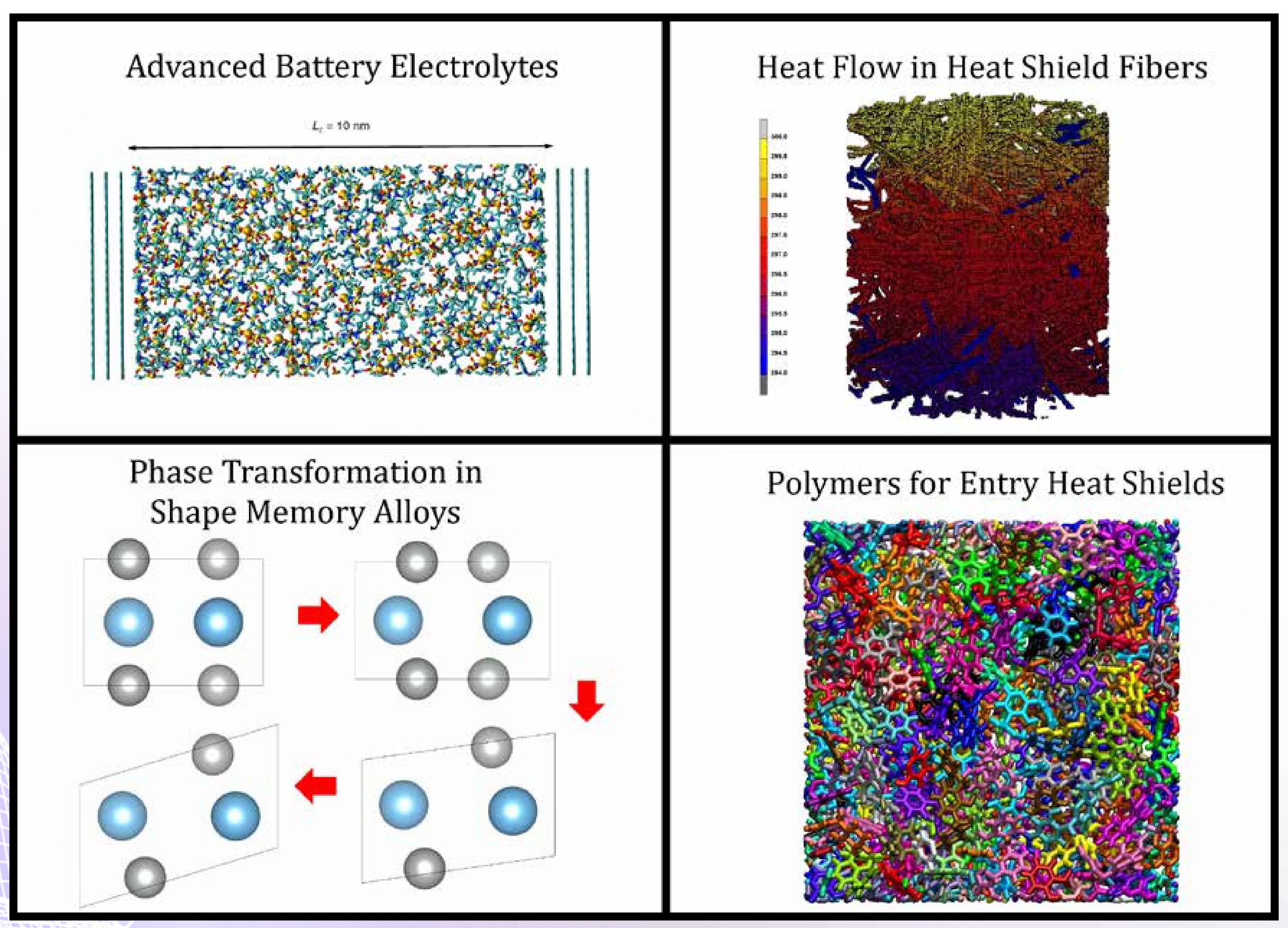
Modeling Materials: Design for Planetary Entry, Electric Aircraft, and Beyond



Multiscale modeling breaks down the elements of material design factors to their relevant time and length scales. The chemistry of a material can be probed with quantum mechanics; its thermal and mechanical properties, with atomistic techniques; and its micro- and macro-scale properties, with continuum methods. As shown in the chart, the output of one level is passed on to the next level, creating a powerful predictive model. *John Lawson, Alexander Thompson, NASA/Ames*



Recent NASA computational materials projects. Top left: Simulation of ionic liquid electrolytes in a nanoscale battery. Top right: Microscale heat flow simulation through fibrous material. Bottom left: Quantum calculations to determine the phases of shape memory alloys. Bottom right: Simulation model of thermoset polymer resin used for ablative composites. *John Lawson, Alexander Thompson, NASA/Ames*

NASA missions push the limits of what is possible. The development of high-performance materials must keep pace with the agency's demanding, cutting-edge applications. Researchers at NASA's Ames Research Center are performing multiscale computational modeling to accelerate development times and further the design of next-generation aerospace materials. Multiscale modeling combines several computationally intensive techniques ranging from the atomic level to the macroscale, passing output from one level as input to the next level. These methods are applicable to a wide variety of materials systems. For example:

- Ultra-high-temperature ceramics for hypersonic aircraft—we utilized the full range of multiscale modeling to characterize thermal protection materials for faster, safer air- and spacecraft.
- Planetary entry heat shields for space vehicles—we computed thermal and mechanical properties of ablative composites by combining several methods, from atomistic simulations to macroscale computations.
- Advanced batteries for electric aircraft—we performed large-scale molecular dynamics simulations of advanced electrolytes for ultra-high-energy capacity batteries to enable long-distance electric aircraft service.
- Shape-memory alloys for high-efficiency aircraft—we used high-fidelity electronic structure calculations to determine phase diagrams in shape-memory transformations.

Advances in high-performance computing have been critical to the development of multiscale materials modeling. We used nearly one million processor hours on NASA's Pleiades supercomputer to characterize electrolytes with a fidelity that would be otherwise impossible. For this and other projects, Pleiades enables us to push the physics and accuracy of our calculations to new levels.

Alexander Thompson, John Lawson, NASA Ames Research Center