The understanding of phenomena from science and of processes from engineering is no longer an exclusive realm of theory and experiment; computation is now regarded as an equal and indispensable partner for the advance of scientific knowledge and for engineering practice. In an important number of cases, computer simulations supplement experiment, but in many others, they are the enabling tool for the study and understanding of complex systems and natural phenomena that would otherwise be too expensive or dangerous, or even impossible, to study by direct experimentation. The study of material properties and processes is one of such areas in which computational science and engineering has become vital. The existence of fundamental theory and methods to describe the behavior of matter at multiple length and time scales, starting from first principles nanometer scale, has made it possible to routinely solve problems that were once thought to be intractable. In spite of these advances, important challenges remain in lieu of the different constitutive equations, models and methods used at each level (scale). Current conventional research theory, technologies and methods cannot characterize or predict complex material properties and processes, dictated from the nanometer scale, with inherently multiscale interactions. “Single image” simulation platforms, integrated from multi-theory, methods, engines and tools, are required to seamlessly and autonomously traverse, in a bidirectional manner, multiple length and time scales. Simulation frameworks that favor such seamless coupling and integration of overlapping models and computational tools across multiple scales are becoming increasingly important for the study of structure and properties of matter in a multiplicity of application fields. This will allow us improve upon, among other things, our ability to design, analyze and interpret experimental results, perform model-based prediction of phenomena, as well as to precisely control multi-scale systems. This brief talk introduces the computational design strategies and implementation issues of such a single-image multiscale simulation platform: The Computational Materials Design Facility (CMDF) currently under development at Caltech’s Materials and Process Simulation Center and at the Massachusetts Institute of Technology.