

1.0 EXECUTIVE SUMMARY

This Critical Review and Technology Assessment was conducted by the Advanced Materials and Processes Technology Information Analysis Center (AMPTIAC), and presents an overview of the tools, techniques and methodologies of utilizing computational tools in the simulation of various materials behavior, properties and implementations. Collectively this is known as computational materials science. Many of the researchers and research efforts across the country are highlighted so that the reader may easily identify areas of relevance. The report should also aid someone new to the field but interested in finding out more, by directing them to references and, in many cases, the leading researchers themselves.

Computational materials science simply is the group of methods that seek to simulate real-world behavior of materials using computer models. At its most basic, it is computing the electronic structure of the atom and how this structure determines bonding and all subsequent properties. At the other end of the length scale is the finite element model, which makes use of constitutive material models and is already widely used in engineering today.

Researchers are utilizing computational tools to design materials and materials systems also. By beginning with the basic building blocks of matter and simulating interactions, some of the tools are able to predict select material bulk properties.

The report is divided into sections that describe modeling and simulation efforts in terms of their length scale. The method of classification is strictly an aid to organizing the topics and is not meant as an endorsement of any particular method over others. Length scale is roughly synonymous with the time interval of the simulation. For instance, the interval of time that is typically simulated in an atomistic computation is on the order of pico- or nanoseconds, while finite element models may simulate seconds. Simulation time is also related to total computational time in the sense that the longer the sampled interval, the more computer processing time will be required.

Other methods are also presented which seek to link the smallest scale problems up through the length scales with multi-scale methods. These average smaller scale contributions into manageable portions, assuring that critical areas are modeled to a finer scale while non-critical areas are smeared and averaged.