“Exascale” computing (10\(^{18}\) floating point operations per second) is commonly seen as the next milestone in the high performance computing world. If this goal can be reached by the year 2020 or shortly thereafter, it will continue the remarkably consistent improvement in computing capability over many years (approximately three orders of magnitude per decade). This astonishing growth has resulted in dramatic changes in all fields in the scale of problem that can be attacked. Materials science is certainly one of them.

Computational materials science focuses on the properties of families of materials, usually with potential technological applications. Computer simulations have obvious advantages when we are dealing with materials that are toxic and/or radioactive, but they have other decisive benefits. Francis Crick\(^{1}\) noted “if you want to study function, study structure,” and calculations of the change of the total energy of the system as a function of the atomic coordinates—the “energy surface”—allow us to determine precisely that. The lowest energy determines the most stable structure, and the form of the surface determines, for example, reaction paths and energies. This structural information can be found directly from the simulation, in contrast to experimental methods of structure determination, such as x-ray and neutron diffraction, or nuclear magnetic resonance. In 30 years of density functional calculations, for example, we have moved from mapping out the energy surface of a molecule as small as ozone\(^{2}\) to performing millions of self-consistent calculations of energies and forces in systems with hundreds of atoms (see below).

Just a few years ago\(^{3}\), I wrote that “materials science is one of the great beneficiaries of changes in the landscape of scientific computing,” but this assessment has proved to be incorrect. Problems in materials science and condensed matter physics in general currently play minor and diminishing roles in present-day allocations of resources of JUQUEEN, compared with elementary particle physics, in particular. No physicist doubts that the latter are crucial to our understanding of the basic structure of matter, and its practitioners often emphasize this “fundamental” aspect. Nevertheless, one of the most eminent of their number, Steven Weinberg, noted how far elementary particle physics is from applications of any sort\(^{4}\).

References

4. “Although surprises are always possible, my own main research area, elementary