Database Tools for Materials Properties

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ABSTRACT

The recent successes of computational chemical methods are well known to the audience at the MSC. These successes have led to the application of these methods to a wider range of problems, incorporating a wider range of parameters, techniques, and analysis tools. The increase in computational power described by Moore’s Law now allows computational chemists to run hundreds of calculations in the same time that formerly was required by a single calculation. These factors have produced an information technology nightmare: more computational chemists running more calculations on more different systems. For a research group with even a handful of computational chemists, it is almost impossible to quickly recover the results of one’s own calculations, much less a coworker’s, at a time when industry and academia are relying on computational chemists to drive research like never before. Clearly, there is a pressing need for high quality database tools targeting computational chemistry.

We are now in the process of developing such tools. Our goal is to archive not only the calculations, but also the properties that derive from these calculations, for quantum mechanical, molecular mechanical, mesoscale, and continuum-level materials properties computations.

We are initially focusing our efforts on developing database tools for the DOE ASCI-ASAP project at Caltech, for which the MSC provides materials properties for both the Solid Dynamics and High Explosive thrusts. Here a wide range of properties are required (bulk moduli and dislocation properties for solids, reaction rates, heat capacities and bulk thermochemical properties for high explosives), and each property may depend upon hundreds of simulations. Reproduction of earlier properties calculations, and update of these properties when new simulations are performed, requires sophisticated database tools.
Our toolkit uses SQL (structured query language) databases, with a variety of web-based and free-standing viewing applications to create, access, and maintain databases of materials properties computations. Figure 1 shows a schematic of the current state of our tools.

In this presentation, we describe the scope of the problem, discuss why database tools are needed, present an overview of the solutions we have developed to date, and discuss future directions of this work.