Software for computational chemistry and materials modeling

Erik Deumens

Quantum Theory Project, University of Florida, Gainesville, Florida 32611

This talk gives a short overview of the evolution of software for computational chemistry and materials modeling over the past 50 years. It then makes a critical assessment of the need for a Scientific Software Innovation Institute for Computational Chemistry and Materials Modeling (S^2 I^2 C^2 M^2). It is argued that the creation of software in the theoretical chemistry and materials physics community is in the artisanal stage and is very successful this way, with training of apprentices by masters to become masters themselves and with many diverse groups brining innovation. However, there is a lot of duplication of work with little spreading of the value provided by the innovation because of lack of software standards. This makes it very hard to tackle the grand challenge problems, like accurate description of super conductivity, prediction of new materials without experimental input, design of novel catalysts. To achieve a production software development environment in which innovative new theories can be rapidly conceived, implemented, tested, and validated requires the community to move to the industrial stage. Software engineering practices, standards for data interchange, quality controls, error estimates are needed to make that possible. Then a new level of innovation can take place.