

PROJECT SUMMARY

This proposal presents an effort to develop a highly scalable suite of coupled cluster (CC) codes. These include the traditional CCSD, CCSD(T) and CCSD[T] methods, as well as the exciting new and novel renormalized, completely renormalized and fully multi-reference methods. The analogous methods for excited states using the equations of motion (EOM) approach will also be made parallel. These accomplishments will be combined with new highly scalable approaches for computing numerical derivatives that are already in place, thereby facilitating the prediction of geometries and vibrational frequencies with the highest levels of theory, for molecules that have not previously been accessible. The methods developed here will find general applicability in a broad range of areas, including organic, biological and materials chemistry.

Broader Impacts: The methods developed here will find general applicability for modeling a broad range of areas, including organic, biological and materials chemistry, as well as many areas of physics and engineering. In addition, the new paradigms that are developed for making parallel codes for highly correlated electronic structure methods will be broadly used as templates for parallelizing the most complex codes used in the physical sciences and engineering. Likewise, the proposed applications are fundamental prototypes that will be of broad interest to the chemical community. More generally, all new developments will be incorporated into the GAMESS suite of electronic structure theory codes, distributed at no cost. The GAMESS user community now numbers in excess of 5,000 users in academia (including both research and undergraduate and graduate courses), government laboratories and industry. New developments in GAMESS are also frequently shared with developers of other electronic structure codes. Finally, Iowa State University is the site of an REU (Research Experiences for Undergraduates) program in Computational Materials Science. GAMESS plays a major role in these undergraduate projects in chemistry, mathematics, and physics.