VIRT&L-COMM.19.2019.19

Cloud Computing ideas on European Open Science Cloud (EOSC)

Grier M. Jones, Department of Chemistry, The University of Tennessee, Knoxville, US

A novel cloud computing application for maximizing the efficiency of quantum chemistry calculations is proposed in order to make quantum chemistry more accessible and efficient for scientists from across the world. The European Open Science Cloud (EOSC) could be used to create an application interfaced with the cloud computing utility that will accelerate accurate electronic structure theory calculations. In essence this utility would recycle wavefunctions and quantum chemical information used in software packages for property determination such as one- and two-electron integrals, Hartree-Fock orbital energies, Fock matrices, molecular and atomic orbitals, and density matrices in order to speed up quantum chemical calculations. For large systems such as calculations with 15+ atoms and a triple-zeta basis set expansion, some of these matrices will be very large. Transferring these matrices will be challenging if not impossible. The software can examine which information to reject or transform and compress for further use. The recyclable quantum chemistry information could have a broad international impact by interfacing with quantum chemical packages such as Psi4 or OpenMolcas.

Instead of restarting all calculations from scratch, users could download information pertinent to their system from the cloud. The quantum chemical information on the cloud would be maintained and verified to insure a high-level of trust and high-degree of accuracy. This utility would allow the users to reduce computational effort and resources that clog up hardware by providing the user with a better initial "pre-conditioned" wavefunction from a variety of traditional or cutting-edge methodologies. The users could call wavefunction information from methods like Hartree-Fock all the way up to expensive methods such as coupled-cluster with singles and doubles and perturbative triples (CCSD(T)), the "gold standard" of quantum chemistry, or multireference methods.[1] By utilizing this information from the cloud, users would not have to reinitialize certain expensive calculations and share information from their calculations that could be upload into the cloud. Our group has already demonstrated the applicability of this scheme for coupled-cluster methods.[2] This could be an open-source initiative to bring quantum chemistry further into the 21st century. This utility could allow users with limited computational resources to perform high level calculations that would take hours or days on a traditional computer, and generate accurate potential energy surfaces in considerably less computational time. It could also be used by data scientists and chemist interested in data-driven and machine learning quantum chemical applications and cheminformatics. The cloud computing-based recyclable quantum chemical resource could be utilized in order to better understand problem applications such as spectroscopy, photochemistry, excited states, drug discovery, materials discovery, and catalyst optimization, with direct applicability in medicinal, materials, green chemistry, and many other applied sciences. Many of these applications are of interest to industry, academia, and governmental organizations that seek to address problems such as greenhouse gas emissions, drug discovery, and catalysis.

Work Cited:

ISSN: 2279-8773

1. Townsend, J.; Kirkland, J. K.; Vogiatzis, K. D. Post-Hartree-Fock Methods: Configuration Interaction, Many-Body Perturbation Theory, Coupled-Cluster Theory. In *Mathematical Physics in Theoretical Chemistry*; 2019; pp 63–117.
2. Townsend, J.; Vogiatzis, K. D., Data-Driven Acceleration of the Coupled-Cluster Singles and Doubles Iterative Solver. *J. Phys. Chem. Lett.*, **2019**, *Just Accepted*. DOI: 10.1021/acs.jpclett.9b01442.

ISSN: 2279-8773