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Computational Chemistry in the Cloud

Gregory Campbell
Hope College

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Gregory Campbell and Dr. William Polik
Department of Chemistry, Hope College, Holland, MI 49423

Introduction

Computational chemistry requires expensive computers and significant computer expertise. The Polik group is remedying these issues by using cloud computing to lower costs and by developing our SITC script to reduce the need for local expertise. In this way, we are making computational chemistry cheaper and more accessible to a wider range of chemistry students and researchers.

Computational Chemistry

Computational chemistry utilizes software to calculate chemical properties and simulate chemical phenomena. Many powerful computational chemistry programs exist.

- Free: Gamess, Mopac, NWchem, Orca, PSI4
- Commercial: Gaussian, Molpro, QChem

Barriers

Unfortunately, there are significant barriers to usage.

- Specialized knowledge is required to operate most computational chemistry programs
- Powerful and expensive computers are needed for intensive calculations
- Local computer experience is necessary to install and set up the software

These barriers are overcome with the WebMO interface, cloud computing, and our SITC installation script

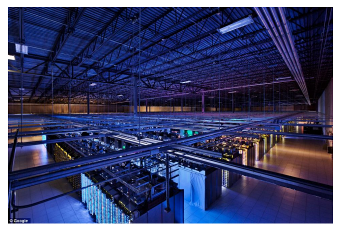
Cloud

The cloud consists of many computers, utilized for storage and computation, housed at sites called server farms. Renting time on the cloud makes high-performance computation much cheaper and more accessible. There are many benefits to cloud computing.

- No up-front costs
- Only rent what and when you need
- Built-in expertise for installation
- Redundancy

However, there are also some drawbacks to utilizing the cloud.

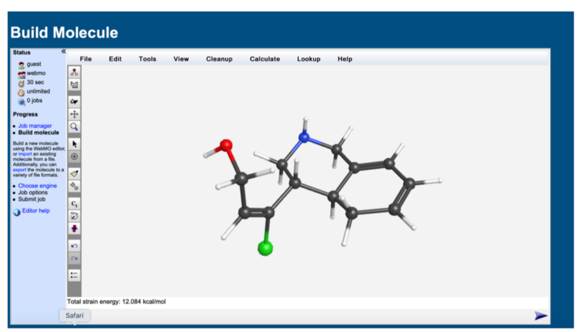
- Need internet connection
- Not cheaper if computing 24 hrs/day, 365 days/yr



WebMO

WebMO makes computational chemistry software more usable for nonexperts.

- A graphical interface replaces the otherwise text-based input and output of computational chemistry programs
- A single interface handles many different computational chemistry programs



SITC

The SITC (Server In The Cloud) script automates the installation of computational chemistry software on the cloud.

- Recognizes cloud vendor and operating system
- Installs text-based computational chemistry programs and WebMO interface
- Configures programs for use

Compatibility

SITC supports multiple cloud vendors, Linux distributions, and computational chemistry programs.

Google Cloud Platform

	PSI4	ORCA	Mopac7	OpenMopac	NWChem	Gamess
Ubuntu	yes	yes	yes	yes	yes	yes
Debian 8	?	?	?	?	yes	?
Debian 9	yes	yes	yes	yes	N/A	yes
Centos 6	yes	yes	yes	yes	yes	yes
Centos 7	yes	yes	yes	yes	yes	yes

Amazon Web Services

	PSI4	ORCA	Mopac7	OpenMopac	NWChem	Gamess
Amzn1	yes	yes	yes	yes	N/A	yes
Amzn2	yes	yes	yes	yes	N/A	yes
Ubuntu	Yes	yes	yes	yes	yes	yes

Improved Access

By eliminating barriers, the Polik group brings computational chemistry to many more people.

- Colleges with limited monetary resources or technical knowledge
- High school classrooms

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