Cloud Services for Reaction Modeling

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Several cloud services have been created and are being developed as shown in multiple areas of chemical information. The development of these services has been primarily created for the domain combustion research, both experimental and modeling. The molecular representation of the modeling is primarily 2D-graphical for the estimation of thermodynamic quantities[2] and the management and automatic generation of combustion mechanisms [3]. For the promotion of FAIR[4] data principles, i.e. that the data be findable, accessible, inter-operable and re-usable, for the promotion of TOP[5], transparency and openness support within journals and for the promotion of the good scientific practices of accountability, traceability and reproducibility the CHEMCONNECT suite of programs strives to manage the data for the whole scientific process from the devices, raw data (modeling and experimental), data manipulation to the final published results. The view of data as not being an isolated point but as a network of interconnections.
The basic services are:

- CHEMCONNECT[6]: This views the information associated with combustion mechanisms as a set of interconnected points using the Resource Description Framework (RDF [])for effient searching.
- CHEMCONNECT2016[8-10]: The database is supplemented by an ontology describing the observations, devices, algorithms and protocols associated with the experimental data.
- JTHERGAS[2,11-12]: This is the quick calculation of thermodynamic quantities (mainly for large mechanisms in combustion research) from 2D-graphical representations of molecules.
- REACTION[3]: This is system for the automatic generation of complex combustion mechanisms (based on 2D-graphical representations of molecules).

Currently, they are being implemented on the Google Cloud Platform, but their software structure is such that they can be ported to other cloud platforms. Each service has their own cloud-based user interface using GWT Material Design in which an interface written in JAVA is transformed into java script. These can be ported using war files to other platforms. On the server side, some of the services are based on the mySQL and Google datastore database systems. In addition, some of the services involve C and C++ code on the server side. These are contained in docker files. Associated with all the services are RESTFUL calls which perform the essential tasks. In addition, the services are individualized using a login (currently using Oauth2 login services of Google, Facebook and LinkedIn) which facilitates personal, consortium and public data.

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