SimplifyGAMESS

EP Analytics is developing a cross-platform solution, SimplifyGAMESS, that aims to lower the barrier to entry of using state-of-the-art quantum chemistry software for academic, commercial, and government research. We were recently awarded with a United States Department of Energy (DOE) Small Business Innovative Research Phase 1 award to develop a proof of concept and prototype of SimplifyGAMESS (https://www.sbir.gov/sbirsearch/detail/1711177).

SimplifyGAMESS consists of a user-centric visual front-end desktop application that provides researchers with access to:

- performance-optimized quantum chemistry applications (e.g., GAMESS, NWChem, PSI4, and TorchANI),
- on-demand cloud HPC resources,
- and centralized tools to create, manage, visualize, and schedule calculations.

The SimplifyGAMESS back-end handles tasks scheduling, software stack maintenance, resource management of local and traditional on-premise HPC, and cloud HPC infrastructure management (e.g., provisioning, configuration, scaling, and teardown). SimplifyGAMESS can reduce or eliminate the overhead related to software maintenance and infrastructure management from researchers. A high-level schematic of SimplifyGAMESS is shown in Figure 1.

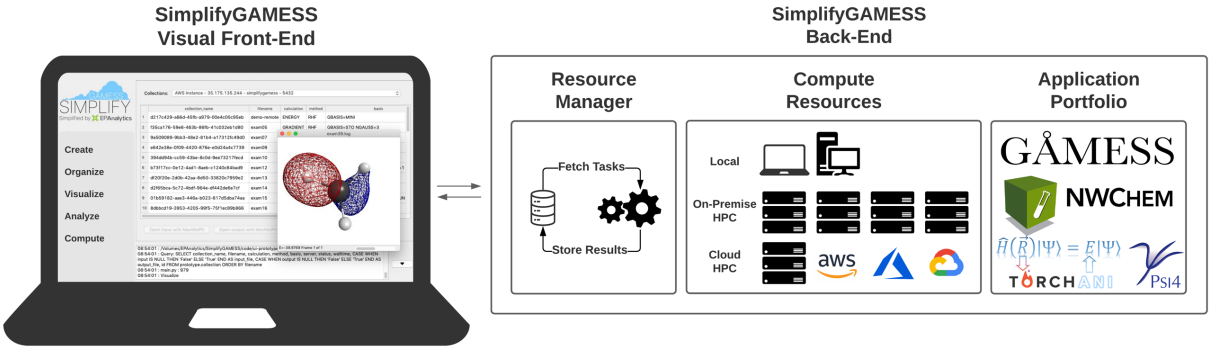

Figure 1. Schematic of SimplifyGAMESS cross-platform infrastructure solution

Our Phase 1 prototype of SimplifyGAMESS is capable of:

- creating GAMESS inputs through the use of the loosely integrated MacMolPlt molecular visualization program, input builder form, and integrated text editor,
- organizing and visualizing collections of GAMESS calculations and extracted metadata,
- supporting in situ data analysis of remote data collections through Jupyter notebooks,
- and scheduling calculations on local, remote, and on-demand computing resources.

A 90-second video showcasing the above capable is available for public viewing at the following location, https://www.youtube.com/watch?v=JwmjCv9LzZ0. A more in-depth 10-minute video is also available, https://www.youtube.com/watch?v=CGTswTHLHHM.

Our plans for Phase II are to expand the capabilities of the SimplifyGAMESS platform and the MacMolPlt molecular visualization tool. For the SimplifyGAMESS platform, we plan to develop in Phase II:

- a **query generator** to enable users to create queries for data collections through the visual front-end,
- a **workflow manager** to enable users to create and schedule data-dependent tasks across available compute resources,
- a **cloud-HPC manager** to handle provisioning, configuring, and scaling on-demand compute clusters in the cloud with a click,
- **traditional HPC** support through the visual frontend to allow users to manage their calculations through a single unified dashboard on the visual front-end,
- and **serverless high-throughput** compute capabilities.

For the MacMolPlt molecular visualization tool, our Phase II plan is to:

- add **automatic molecular fragmentation** capabilities to support input generation for the fragment molecular orbital (FMO) and effective-fragment molecular orbital (EFMO) method,
- support **molecular orbital visualization** across multiple points **along** a **reaction path** in a single view,
- add **solvation capabilities** with ab initio and the effective fragment potential (EFP) method solvents,
- add **native support** for the Molecular Science Software Institute (**MolSSI**) Quantum Chemistry (**QC**) **JSON schema**,
- and extend the **command-line interface** capabilities.

We feel that our SimplifyGAMESS platform will enable researchers across diverse molecular science domains to utilize salient features within our performance-optimized quantum chemistry application portfolio to leverage powerful capabilities such as the linear-scaling FMO and EFMO methods in GAMESS to accelerate innovation.

The principal investigator (PI) in the SimplifyGAMESS project is Dr. Sarom Leang, who brings experience in both computational chemistry and cloud technologies. Dr. Leang received his Ph. D. from Iowa State University under the mentorship of Dr. Mark Gordon (PI of GAMESS). Dr. Leang is currently the development lead of GAMESS.

EP Analytic is a small business based in San Diego, California founded by leading researches in the performance analysis, modeling and characterization of higher performance computing systems. EP Analytics assists clients in the government and private sector in designing and procuring mission-critical HPC systems and maximizing the effectiveness and energy-efficiency of existing systems based on specific application characteristics. With the increasing reliance on modeling & simulation, virtual prototyping, and computer-aided engineering across numerous market segments, EP Analytics' expertise and tools can assist enterprises in maximizing the return-on-investment in HPC systems.