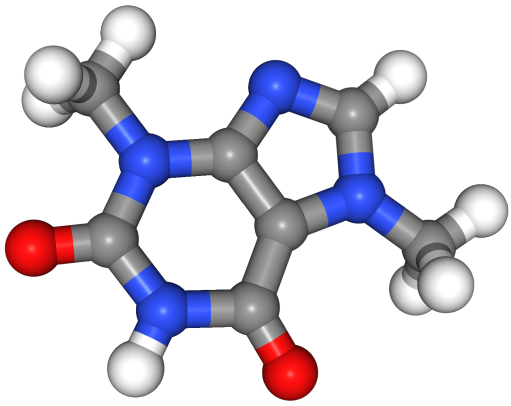
SEAMM

A Simulation Environment for Atomistic and Molecular Modeling

SEAMM is a user-friendly software package for the atomistic simulations of organic molecules, fluids, and materials such as metals, metal oxides, semiconductors, ceramics and alloys. SEAMM is an ideal environment for discovery and production, helping you focus on the science instead of getting bogged down in the details of how to run the software.

Installing SEAMM

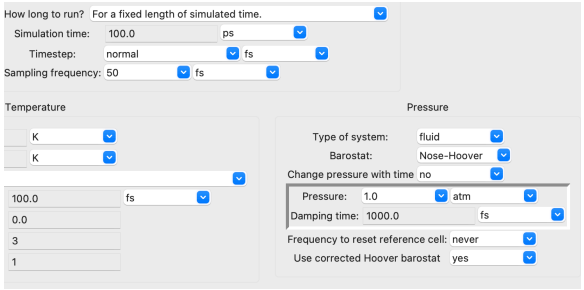
SEAMM and other simulation engines such as LAMMPS, DFTB+, Psi4, and Packmol are conveniently installed on Linux or Mac operating systems, with support for Windows coming soon.



User Experience

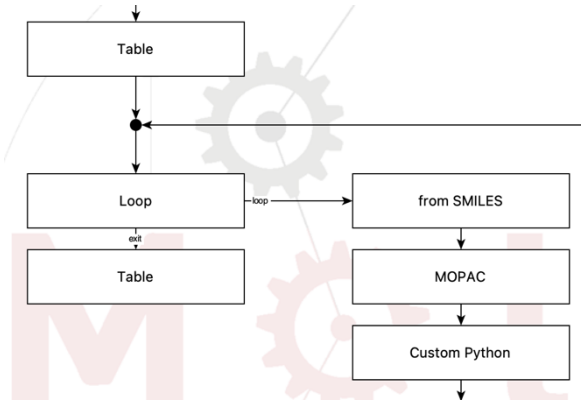
SEAMM arms users with a graphical user interface (GUI) that exposes its full power and functionality in a user-friendly environment. The GUI removes the need to learn verbose, complicated keywords and code-specific syntaxes. Furthermore, the GUI employs reasonable defaults for most parameters, so you can start quickly with your simulation and get reasonable results even for codes that you haven't used before.

As you learn more about the details of each model and the corresponding tools, you can further customize your calculations to tailor them to your specific problem.



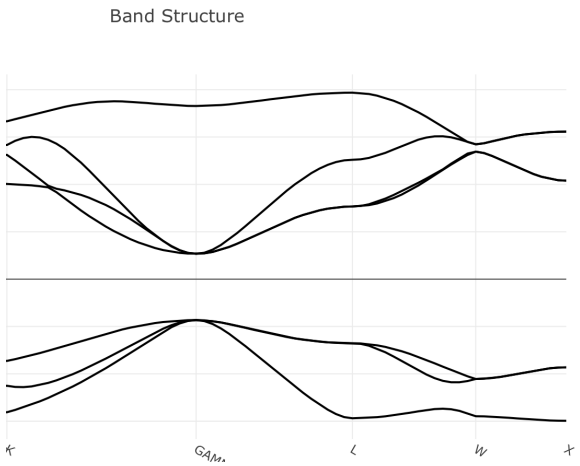
Reproducibility

Flowcharts are a foundational concept in SEAMM offering a high-level and intuitive delineation of the entire workflow.



Flowcharts remove the need for shell or python scripting while making the entire process reproducible. If you re-run a

flowchart, it will do exactly the same calculations and produce identical physically meaningful results. While flowcharts are critical for enforcing reproducibility, they are editable, allowing users to perform necessary tweaks and changes to the workflow. For example, the same set of calculations within a flowchart can be performed on a variety of molecules and materials without any further changes. In a different scenario, changing parameters is easily accommodated in an existing flowchart. For example, fine-tuning the pressure or temperature variables in a simulation. Flowcharts make all these changes convenient and reproducible.



Share your work

Because flowcharts are simple text files, they can be easily shared with coworkers and collaborators. This means you can get flowcharts from experts in areas that are outside your area of expertise and use them as a starting point for your studies.

You can publish flowcharts to Zenodo directly from SEAMM, and get a unique DOI. With SEAMM, you can search for and import flowcharts directly from Zenodo.

Track your work

SEAMM provides a datastore and web-based dashboard for storing, monitoring, and managing the calculation results. The datastore organizes each project in a separate directory on disk and provides well-structured results that are easily monitored and managed using the dashboard.

Manage your data

Most funding agencies require a data management plan for the dissemination of scientific data. With SEAMM, you publish your computational campaigns via the dashboard and will be able to publish results directly to Zenodo, uploading the data and generating a unique DOI in a few clicks.

Manage your citations

SEAMM helps you gather the appropriate citations for the codes and parameter sets used in your computational campaign. Each job creates a list of references for the current task and stores it in a database. We are developing tools to allow merging all the citations from a single computational campaign into a single list.

For further details about SEAMM see the documentation at https://molssi-seamm.github.io