FHI-aims Input Generator for Avogadro 2

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Overview

Avogadro 2 is an open-source chemical editor and visualization tool used in computational chemistry, molecular modeling, bioinformatics, and materials science. It is a rewrite of the original Avogadro software in order to offer more flexibility and greater extensibility by enabling the integration of Python scripts to add simulation input capabilities as well as data input and output. One of the main aspects of Avogadro 2 is the shift from Qt/C++ to Python for creating input generators. This project utilizes this feature to create an FHI-aims input generator that exports a "geometry.in" text file containing the spatial information of a molecule in a format that is recognizable by the FHI-aims package. In this project, the Python script "aimsinput.py" was created using the Spyder IDE. The steps below, written for MacOS, outlines the process of integrating this script into Avogadro 2 and activating the FHI-aims input generator plugin.

1 Downloading Avogadro 2

The latest version of the Avogadro 2 build (1.93.0) can be downloaded from `https://github.com/OpenChemistry/avogadrolibs/suites/648275435/artifacts/5525298`. If this link is not working, the file "Avogadro2-1.93.0-Darwin.dmg" can also be found at `https://drive.google.com/drive/folders/1jikKel3LIVc26og62gRURPhYPdTQqy2u?usp=sharing`

2 Downloading the "aimsinput.py" File

A copy of the python script for the FHI-aims input generator can be found at `https://github.com/frda058/ColumbiaMRSEC`. If this link is not working, the file is also available on the Google Drive link above. Save this file on your computer.

3 Accessing the Avogadro 2 Package Contents

Once Avogadro 2 is downloaded, go to the computer's Applications folder. Right-click (or control + click) on Avogadro 2 and click on "Show Package Contents" →"Contents" →"lib" →"avogadro2" →"scripts" →"inputGenerators". This folder will contain the python scripts for the available input

generators such as Dalton, GAMESSUK, and Gaussian. Copy and paste the "aimsinput.py" file into this folder.

4 Opening Avogadro 2 and Setting Python Path

Open Avogadro 2. If this is the first time the application is being accessed and an error message appears, go to Finder →Applications. Right-click (or control + click) on Avogadro 2 and click "Open". Since input generators are written in Python, Avogadro needs to know which Python interpreter to use. To do this, click on "Quantum" →"Input Generators" →"Set Python Path". To determine where the Python path, go to the Terminal and type the following command (without the $ sign and using single spaces):

```
$ which python3
```

Copy the output and paste it onto the Avogadro prompt to set the path. If you don't have the most recent version of Python 3, refer to the Downloading Python 3 section below.

5 Building a Molecule and Optimizing Geometry

Restart Avogadro 2 and build the molecule of interest. If this is the first time the application is being accessed and an error message appears, go to Finder →Applications. Right-click (or control + click) on Avogadro 2 and click "Open". To optimize the molecule's geometry, click on "Extensions" →"Open Babel" →"Optimize Geometry". If there are error messages regarding Open Babel, please refer to the Open Babel section of this document to fix the issue.

6 File Export

When the molecule is created, click on "Quantum" →"Input Generators" →"FHI-aims". Use the name of the molecule as the title and the filename base. This input generator will save two files – a "geometry.in" text file that is ready to be imported into the FHI-aims package and another text file with a file name containing the name of the molecule (ex. "piperazine.txt"). The second file is created to keep a record of the spatial information generated for each molecule and can easily be accessed on the computer. The contents of the two files, however, are the same. Afterwards, click on "Write files to disk" and select the folder that the text files will be saved in.

Issues with Open Babel for Optimizing Geometry

When optimizing the geometry of the molecule, a message stating "Error interpreting Open Babel Output" may occur. The following steps were performed to resolve the issue for MacOS.

1 Installing Homebrew and CMake

Homebrew is a package manager that simplifies the installation of software on Apple's macOS operating system. It can connect to repositories and download different programs using the Terminal. To download Homebrew, type the following command in the Terminal:

```
$ /bin/bash -c "$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/master/install.sh)"
```

CMake is requirement for downloading Open Babel and can be downloaded using Homebrew. To do this, type the following command in the Terminal:

```
$ brew install cmake
```

2 Installing Open Babel

Open Babel (version 2.4.1) can be downloaded as a zip file from `https://sourceforge.net/projects/openbabel/files/latest/download`. The basic build procedure is conducted at the Terminal. The file will be saved in the Downloads folder. Do not open and unzip the file. In the Terminal, type the following commands:

```
$ cd Downloads
$ tar zxf openbabel-2.4.1.tar
$ mkdir build
$ cd build
$ cmake ../openbabel-2.4.1
$ cmake ../openbabel-2.4.1 -DCMAKE_INSTALL_PREFIX=~/Tools -DCMAKE_BUILD_TYPE=DEBUG
$ make
$ make install
```

To create a local build:

```
$ cmake ../openbabel-2.4.1 -DCMAKE_INSTALL_PREFIX=~/Tools/openbabel-install
$ make && make install
```

3 Replacing the obabel Unix Executable File

1) Go to the Finder toolbar at the top of the screen and click on "Go" →"Home". Open the "Tools" folder and click on "openbabel-install" →"bin". Locate the obabel Unix executable file.

2) In a new Finder window, find the Applications folder and open Avogadro 2's package contents. Right-click (or control + click) on Avogadro 2 and click on "Show Package Contents" →"Contents" →"MacOS". Here, you should see another obabel Unix executable file.

3) Replace the obabel Unix file in Avogadro 2 by copying and pasting the obabel Unix file from the bin folder in Step 1 into the MacOS folder of Avogadro 2 from Step 2.

4 Replacing Files with the .so File Extension

1) Open the "Tools" folder again from the "Home" folder as in Step 2.1. Click on "openbabel-install" →"lib" →"openbabel" →"2.4.1". Select all the files in this folder with the .so file extension and copy all the items (right click + copy / command + C).

2) Open Avogadro 2's package contents. Click on "Contents" →"lib" →"openbabel". Replace all the files in this folder with the .so file extenstion by pasting the .so files from Step 4.1 into this location.

3) Open the Avogadro 2 software and test the Optimize Geometry function.

Downloading Python 3

A recent version of Python 3 is required for the input generator plugin. This can be installed using Homebrew. To do so, type the following command in the Terminal:

```
$ brew install python
```

Supplemental Information

- The developers' detailed justification for the Avogadro rewrite can be found at `https://blog.kitware.com/avogadro-2-and-open-chemistry/`
- An article about the the new input generator framework in Avogadro 2 is found at `https://blog.kitware.com/new-input-generator-framework-in-avogadro-2/`
- The build procedure for Open Babel is found at `https://open-babel.readthedocs.io/en/latest/Installation/install.html`. Some steps were modified for Open Babel version 2.4.1.
- The python script for the FHI-aims input generator is always avaialble at `https://github.com/frda058/ColumbiaMRSEC`. Alternatively, it can also be found at `https://drive.google.com/drive/folders/1jikKel3LIVc26og62gRURPhYPdTQqy2u?`usp=sharing
- Python scripts for other input generators can be found at `https://github.com/OpenChemistry/avogenerators`