AutoGaussian: Automated Gaussian Calculation Pipeline for Ground and Excited States in Solution

AutoGaussian is a Python script designed to automate Gaussian calculations for multiple molecules, focusing on ground and excited states in solution. It streamlines the process of running batch calculations with customizable steps, making it ideal for computational chemistry research. This script is specifically designed for calculations using the Polarizable Continuum Model (PCM) to simulate solvent effects, but can be adapted for other SCRF methods.

Key Features

1. **Multi-format Input Support**: Processes .xyz, .com, and .chk files.
2. **Customizable Calculation Steps**: Users can define and order specific calculation steps.
3. **Concurrent Processing**: Allows simultaneous calculation of multiple molecules.
4. **Solvent Environment Modeling**: Implements SCRF (Self-Consistent Reaction Field) calculations.
5. **Flexible Configuration**: Easy adjustment of memory, processors, and Gaussian commands.

Functionality

- The script automatically processes all .xyz, .com, and .chk files in the input folder.
- It applies the same charge and multiplicity to all molecules and executes the same calculation steps for each.
- For the first step:
    - If using a .chk file, the input MUST include "Geom=Check Guess=Read".
    - For .com or .xyz files, these keywords MUST BE OMITTED in the first step.
- Subsequent steps always HAVE TO include "Geom=Check Guess=Read", since they automatically utilize the .chk file from the previous step.
- Users can limit the number of concurrent calculations to avoid overloading queue systems.
- Calculation steps and their order are fully customizable.

Theoretical Background

- This script leverages the Polarizable Continuum Model (PCM) to simulate solvent effects in molecular calculations. PCM treats the solvent as a continuous dielectric medium, allowing for the efficient modeling of solvation effects on molecular

properties. For more information on PCM, refer to the Gaussian documentation: https://gaussian.com/scrf/

Configuration

- Set memory allocation and number of processors.
- Define specific Gaussian commands for each calculation step.
- Select which steps to execute and in what order.
- Set the maximum number of concurrent molecule calculations.

Process Overview

1. Reads input files from the specified folder.
2. Creates standardized .cmxyz files for Gaussian input.
3. Executes defined calculation steps for each molecule.
4. Monitors log files for completion or errors.
5. Manages concurrent processing of multiple molecules.

Requirements

- Python 3.x
- Gaussian 16 (g16 command accessible in system PATH) (also modifiable to g09)

Usage

1. Place input files (.xyz, .com, .chk) in the 'input' folder.
2. Adjust configuration parameters in the script if needed.
3. Run the script: sbatch AutoGaussian.py

This script is ideal for researchers and computational chemists working with multiple molecules and requiring consistent, automated Gaussian calculations for ground and excited states in solution environments.