MSD Software Documentation

Audiences: (1) End Users, and (2) Developers

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# 1. Overview

## (1a) Purpose:

This software suite allows for the study of theoretical (simulated) behavior of **Molecular Spintronics Devices** (MSDs).

## (1b) Intended Audience:

The first part of this document (sections 1-5) are targeted towards “end-users”: e.g. students, engineers, or scientists.

The second part (sections 6-10) provide further details and documentation important for software developers.

## (1c) Background Information:

From Wikipedia, “**Spintronics**, also known as spin electronics, is the study of the intrinsic spin of the electron and its associated magnetic moment, in addition to its fundamental electronic charge, in solid-state devices.”

Traditional **Spintronics Devices** are created by layering two ferromagnets, polarized either parallel or antiparallel to each other, with a spacer or buffer layer between that prevents magnetic coupling. The resistance of the device is then measured and its strength will depend on the magnetic moment of the two ferromagnets. This effect is known as magnetoresistance.

Our lab’s novel **Molecular Spintronics Devices** (MSDs) are similar to a tradition spintronics devices; however, additional complex molecules are sandwiched between the ferromagnets creating only a partial spacer. Some coupling between the ferromagnets and molecules can occur.

The properties of such a device are experimentally varied, and largely dependent on the particular properties of the molecules and other materials used. Given the difficulty and expense required to fabricate a large quantity of various devices for study, theoretic predictions are a great asset. Moreover, by simulating such devices, information about the internal state of the device, data which would be difficult or impossible to measure, can be predicted leading to a deeper understanding of the observed macro-behaviors.

This software uses well know and empirically tested equations and models for calculating energy along with an algorithmic technique know as a Monte Carlo simulation. For more info, see section: [4. Technical Details](#_4._Technical_Details).

# 2. Setup

### (2a) Supported Platforms:

Currently the only platform supported entirely out-of-the-box is Windows (64-bit). The programs have been tested with the latest version of windows (Windows 11 at time of writing), but previous versions of Windows should work as well. There are x86 (Windows 32-bit) versions of some of the programs, but not all.

Although the software is currently targeting a Windows environment, it is written in cross-platform code and can be compiled for and run on any operating system.

### (2b) Download:

The latest version of the software can be downloaded from <https://github.com/Mathhead200/Molecular-Spintronics-Research-Project>. The GitHub archive also contains many previous versions of the software. Check the README file (and/or dates) to see which version is the most resent.

The folder suffixed “Latest Development Version” is the working folder for active development and generally not stable or ready for release. It may contain temporary development files, uncompiled code, broken code, bugs, inefficiencies, and other artifacts of the development process.

### (2c) Install:

There is currently no installer. Just download the desired version (i.e. folder) from GitHub or another distribution source, and unzip (if necessary). The folder titled “MSD Research Project (v\*.\*.\*), …” represents the root folder for the software.

### (2d) Update:

Periodically check the GitHub repository for updates. There is no official update schedule or automatic update tool at this time.

# 3. Run

### (3a) File Structure:

In the root project folder (denoted: ~), you will find a list of files and folders:

#### Files:

* **~/change-log.txt**: This text file provides a detailed history of changes throughout the many versions of this software, including bug-fixes, optimizations, and additional functionality. This is the file to consult if you are not sure what version of the MSD software to use.
* **~/\*.bat**: These batch files are used to run the various C++ applications (apps) provided with this software. Further details about these apps will be provided later in this section.
* **~/parameters-\*.txt, ~/extract-input.txt**: These parameter (plain/text) files are used by their respective apps. Details about how to modify and use them will be provided later in this section along with their respective apps.
* **~/mmt\_compiler.exe**: This app compiles .mmt (MSD Molecule Text) files into .mmb (MSD Molecule Binary) files. This tool is used in conjunction with the mol-builder, and some of the provided apps. More details can be found later in this section.
* **mol-builder.html**: This web app is used to build custom molecules. Details on it’s use are given later in this section.

#### Folders:

* **~/bin**: (*Not for end-users.)* These are where the compiled binaries are stored. More information for developers can be found in section [6. File Structure](#_6._File_Structure).
* **~/dev-tools**: (*Not for end-users.)* This folder contains miscellaneous utilities useful for developers.
* **~/docs**: This folder contains the current documentation for this software.
* **~/lib**: (*Not for end-users.)* This folder contains any ports or binding of the MSD software. More information for developers can be found in section [6. File Structure](#_6._File_Structure).
* **~/mol**: This folder is provided for end-users to store their custom molecules in. Its use is optional. More details about custom molecules are given later in this section.
* **~/out**: This folder is the default output location for apps. This is where the data from the various simulations will be stored when using the apps’ default configurations.
* **~/src**: (*Not for end-users.)* This folder contains almost all the source code for the core MSD libraries and apps. The only exceptions may be tools/libraries written in scripting languages stored directly in ~ or ~/lib. More details for developers in section [6. File Structure](#_6._File_Structure).

## (3b) Iterate

## (3c) Heat

## (3d) Magnetize

## (3e) Magnetize2

## (3f) Metropolis

## (3g) Molecule Builder

# 4. Technical Details

# 5. Acknowledgments

# 6. File Structure

# 7. Abstractions

# 8. MSD Library

# 9. Compiling

# 10. Other Tools