McPherson Monochromator Control Software

User Manual

20 July 2023
Revision 2 for MMCS v0.8

McPHERSON

Contents

> **WARNING:**
> Read and understand this user manual before using the McPherson Monochromator Control Software. Read and understand the user manuals for each device the McPherson Monochromator Control Software can control prior to using or operating the device. Failure to follow the instructions within each manual could result in a dangerous situation.

Important Notices

> **ELECTRICAL HAZARD:**
> Electrical equipment can be hazardous if not handled properly. It is important to ensure that all electrical instruments are used with appropriate grounding on power lines, and that electrically powered components are not manipulated or touched unless they have been switched off and disconnected from the power source.
>
> This notice is reiterated in 5.4 Important Notice Regarding Electronics.

> **DANGER:**
> Mechanical equipment can cause injury if interacted with while in motion. All equipment must be powered down prior to any physical interaction with the equipment.

> **WARNING:**
> In an emergency, the power should be disconnected from the device. Do not rely on the software in an emergency.

> **NOTICE:**
> McPherson Inc. will not be held liable for any harm or damages caused by the equipment if the instructions contained in the respective manual(s) are not properly followed, or if the repairs are performed by personnel who are not trained or licensed by the company. It is the user's responsibility to follow all instructions and use the equipment in accordance with the manufacturer's guidelines.

Please see 5 License and Legal Information for software-related disclaimers and legal information.

1 Introduction

1.1 Overview of MMC Software

The McPherson Monochromator Control Software (MMCS, or "the software") is designed as a modern replacement for the original software, McPherson Spectrometer Control Software, written in LabVIEW. MMCS is developed as an open-source project and welcomes contributions adherent to the GNU Public License v3.0 and 7 How to Contribute. The project is hosted at github.com/mcpherson-inc/MMC, where the most recent source code, executable, documentation, and user manual is available. This software is offered free of charge without any warranties or fitness for a particular purpose.

1.2 System Requirements

The software executable requires the use of Windows 7 or 10, 64-bit; it is important to note that as of the time of writing the executable has been validated exclusively on Windows 10 64-bit. The code can be compiled and run on any environment capable of running Python 3.9.7, although other versions of Python may work. Due to its use of Qt5, MMCS's additional hardware and software requirements derive from Qt5 (qt.io) and PyQt5 (riverbankcomputing.com/software/pyqt/). For more information about running the

program without the executable or interacting with the source code, please see .

1.3   Supported Instruments and Models

The software supports the following instruments from McPherson:

- Monarch (URL TBD)

The software is capable of controlling the following motion controllers:

- ThorLabs KST101 K-Cube Stepper Motor Controller
- McPherson Model 789A-4* (mcphersoninc.com/pdf/789A-4.pdf)
  *Some older models do not have a home switch and are incompatible.
- McPherson 792 (mcphersoninc.com/pdf/792.pdf)

The software is capable of operating the following detectors:

- Keithley Model 6485 Picoammeter

1.4   Getting Started

1.4.1   Downloading and Running

There are multiple options for downloading MMCS. All versions of the software are available on the releases page at github.com/mcpherson-inc/MMC/releases. Expanding the *Assets* dropdown will reveal the executable and zipped source code downloads.

Executable

The executable file *mmc.exe* is included within the *MMCS* zip file. The zip file should be downloaded, its contents extracted, and the MMCS folder placed wherever is most convenient.

The program can be run at any time by double-clicking on *mmc.exe* and does not require installation.

Source Code

The source code can be downloaded either by downloading the *Source code (zip)* file and extracting its contents or by cloning the github.com/mcpherson-inc/MMC repository.

Python is required to run the program from source code. This can be done by opening a Python interface in the program directory and executing `python mmc.py`.

Compilation

The source code can also be optionally compiled and then run. This can be done in one of two methods: one-file and one-directory. The one-file method will produce one executable which is smaller, but slower at

startup. The one-directory method creates a directory of files which is larger, but significantly faster to start. See the `requirements.txt` file, included with the source code, for the required Python modules. Detailed compilation steps are listed below.

Compilation Instructions - One File

    `pipenv run pyinstaller mmc.spec`

    Outputs MMC/dist/mmc.exe

Compilation Instructions - One Directory

    Prerequisites:

    PyQtWebEngine, pipenv

    `pip install PyQtWebEngine`
    `pip install pipenv`

    Pipenv Setup:

    `cd MMC`
    `pipenv install requests`

    Compilation:

    `pipenv run pyinstaller mmc.spec`

    Outputs MMC/dist/MMCS/MMCS.exe

1.4.2   On Startup

The program will, on startup, perform a number of tasks:

1. Create *config.ini* within the program's directory if one does not already exist, or if it is improperly formatted.

2. Present the user with the Device Manager window.

Once the communication ports and connected devices have been selected, the *Accept* button has been pressed, and the program has successfully established communication with the devices, the Main Window will be shown and the Device Manager will be automatically closed. See 2 User Interface for additional details.

2   User Interface

2.1   Device Manager

The Device Manager is the first window that will be presented after starting the MMCS. It is split into two primary sections labeled *Detectors* and *Motion Controllers*. Additionally, at the bottom of the window is an *Accept* button, which begins device connection and launches the main user interface window, and a loading bar, which can be used to monitor the current device connection progress.

Within each primary section is a spin-box input and two drop-down menus. The spin-box value indicates how many detectors or motion controllers should be connected. A maximum of two detectors and 32 motion

controllers is currently allowed. The drop-down menus should then be used to select the communication port for the device (left) and the type of device which is connected to that port (right).

Once the correct device configuration is selected, press the *Accept* button to begin device connection and main interface boot-up.

2.2   Main Interface Window

Once all of the devices are successfully connected, the Device Manager will close and the Main Interface Window (or Main Window) will open. The Main Window is split into the following four distinct sections: a scrollable device control area in the top left, a record of all data collected during this session in the bottom left, a graph of collected data on the right, and a status area in the bottom. Additionally, this window has a menu bar (File, Edit, View, About, and Help) along the top.

2.2.1   Device Control Area

The device control area, located in the top left section, is likely to be the area most frequently used. Here the user is able to control and configure all connected devices. This scrollable area is broken up into the four main axes: *Main Drive*, *Filter Wheel*, *Sample*, and *Detector*. At the top of this area is a bar which is always visible containing the *All Stop* and *Device Configuration* buttons.

The *All Stop* button will immediately halt all device movement. However, if it is used, any axes which were moving at the time will need to be homed, since the position they stopped at is unknown. In an emergency, the power should be disconnected from the device. Do not rely on the software in an emergency.

> **NOTICE:**
> MMCS version v0.8 does not currently support the McPherson Model 747 Device Controller, which is necessary for filter wheel control. As a result, software-directed filter wheel control capabilities are not available in this version.

Above and to the right of the axis controls is a *Machine Configuration* button. This opens a window which allows configuration of the connected device(s) and is discussed further in section 2.2.2 Machine Configuration Window.

Each axis area has a similar layout. At the the top is the title of the area, flanked on the right by a drop-down menu followed by a button.

The drop-down menu provides the ability to quickly change which port controls which axis. Please note that the ports shown in the Main Window includes sub-ports. This means that devices which have the capability of controlling multiple motors will be shown multiple times with a number appended to their name. The port selection discussed here is the same as is found within the Configuration Window, discussed later.

To the right of the port selection drop-down is a area-collapse button, which will display "v" when the area is shown, and "<" when the area is hidden.

Below the axis area title contains the axis-specific controls which enable movement, scanning, and data collection. Manual movement requires entry of the desired resultant position in units, which are marked, in either nanometers or degrees. Pressing the *Move* button will initiate a move to the entered location. The *Home* button is also available to home an axis at any time.

> **WARNING:**
> Motion-sensitive user interface elements are disabled while a movement has been initiated. No attempt
> to initiate further movement should be made while the device is in motion. Press the *All Stop* button
> at any time to halt all movement on the machine. In the unlikely event of a program failure, crash,
> hang, or other form of communication failure, the HALT command may be delayed or lost; the power
> to the motors should be disconnected safely to avoid damage or injury.

Scans are available in the Main Drive, Sample, and Detector axes, and require three input values: *start*, *stop*,
and *step*. Once the *Begin* button is pressed, the scan will begin. During the scan the device is commanded
to move to, and sample at, a number of locations determined by *start*, *stop*, and *step*. Location values
are generated within the closed interval [start, stop] with spacing between values given by *step*. The
scan includes both the starting and ending positions. Additional scan types *Rotation*, *Translation*, and
Theta2Theta are available in the *Sample* axis. Finally, the *Repeats* spin-box can be set to however many
additional and identitcal scans the user would like to do after the first.

2.2.2   Machine Configuration Window

The Machine Configuration Window (or Config Window), which is accessed by pressing the *Machine Con-
figuration* button above and to the right of the axis controls, is necessary for configuring the specifics of
the connected device(s). When pressed, the Config Window will be opened. The Config Window has the
following five tabs: Model, Main Drive, Filter Wheel, Sample Movement, Detector Rotation. The final four
tabs correspond to the axes discussed in section 2.2.1 Device Control Area, but additional input parameters
to set movement limits, grating density, and device model.

To properly set the steps per nanometer value, the model must be selected, grating density entered, and the
Calculate Steps per Nanometer button must be pressed prior to closing the window via the *Accept* button.

The Model tab allows the quick loading of a model-specific device configuration. Please note that loading a
configuration will overwrite all current values and a configuration save should be made to preserve current
values. This is discussed further in section 2.2.6 Menu Bar.

2.2.3   Data Record

The Data Record area lists each scan that has been taken during the current session, enumerated by its
start, stop, and step values. The name given to a scan can be changed at any time by clicking on the name
box. Additionally, the *Plot* column allows toggling the viewability of a scan on the graph. Data can be
deleted by first selecting its entry and then pressing the *Delete Data* button. Likewise, data can be saved
by selecting its entry and then pressing the *Save Data* button.

2.2.4   Data Graph

The plot automatically shows all scans completed during the current session. Which scans are shown is
controlled by the Data Record, discussed in section 2.2.3 Data Record. The *Clear Plots* button can be used
to quickly hide all plots.

2.2.5   Status Area

The Status Area shows, from left to right, the current Main Axis position in nanometers, the system status,
and a progress bar detailing the completion progress of the current scan.

2.2.6 Menu Bar

The menu bar, located at the top of the Main Window, contains a number of useful utilities and settings. The buttons, options, and descriptions are listed below.

- File
    - Export Config: *Exports the current configuration and input values as a CSV file.*
    - Import Config: *Allows selection of a CSV file which will populate the configuration and values.*
    - Save Current Config: *Saves the current software and device configuration*
- Edit
    - Machine Configuration: *Alternative method to open the Config Window (2.2.2 Machine Configuration Window).*
    - Invert measurements?: *Multiplies all future measurements by -1.*
    - Auto-log data?: *Automatically saves all scan data to UNIX-timestamped CSV files.*
    - Change Auto-log Directory: *Change where auto-logged data is saved.*
    - Preferences: *Unimplemented.*
- View
    - Pop-out Plot: *Unimplemented.*
    - Pop-out Table: *Unimplemented.*
    - Show Main Drive: *Unimplemented.*
    - Show Filter Wheel: *Unimplemented.*
    - Show Sample Movement: *Unimplemented.*
    - Show Detector Rotation: *Unimplemented.*
    - Show Data Table: *Unimplemented.*
- About
    - Source Code: *Opens a link to the GitHub repository.*
    - Licensing: *Opens a link to the GitHub repository.*
- Help
    - Manual: *Opens a link to the GitHub repository.*

3 Features and Functions

3.1 Data Management

3.1.1 Saving and Loading Data

Saving and loading collected scan data is covered in section 2.2.3 Data Record.

3.1.2 Importing and Exporting Configurations

Exporting and importing configurations and values is covered in section 2.2.6 Menu Bar.

3.2 Data Visualization

All data is visualized using the Data Graph discussed in section 2.2.4 Data Graph.

4 Troubleshooting and Support

4.1 Error Messages

Following are lists of known error messages and their probable causes. Any messages received which are not listed here should be reported via the process detailed in 7.1 Reporting Bugs. Crashes should also be reported. In Table 1, the "Sev." column notes the severity of the issue. INFO indicates an informative message which does not require significant action. WARN indicates an issue that does not require the program to be restarted. CRIT indicates an issue that can likely only be fixed by restarting the program.

Errors 4-7 report an additional message, represented by the %s. These may provide additional insight into the cause of the issue.

Table 1

Errors			
#	Title, Message	Sev.	Possible Causes
1	Connection Failure No detector was selected for entry #%d.	INFO	Detector not selected.
2	Connection Failure No motion controller was selected for entry #%d.	INFO	Motion controller not selected.
3	Connection Failure Connection attempt has failed!	WARN	Devices are not connected properly.
4	Move Failure Main drive axis failed to move: %s.	CRIT	Communication or connection failure.
5	Move Failure Sample rotation axis failed to move: %s.	CRIT	Communication port fell asleep. Device disconnected.
6	Move Failure Sample translation axis failed to move: %s.	CRIT	Communication port fell asleep. Device disconnected.
7	Move Failure Detector rotation axis failed to move: %s.	CRIT	Communication port fell asleep. Device disconnected.

4.2 Common Issues

We look forward to updating this section with feedback from users.

4.3 Contacting Support

When encountering issues with the software, we recommend visiting github.com/mcpherson-inc/MMC/issues first. However, we strive to provide our customers with the best support possible, and we are always happy to help. If you have any questions or concerns, please don't hesitate to reach out to us. We are available Monday through Friday, from 9:00 AM to 5:00 PM Eastern Time.

Please see 6.2 Contact Information for details.

4.4 Updating the Software

Updating the software requires downloading the latest version found at github.com/mcpherson-inc/MMC/releases and following the instructions in 1.4.1 Downloading and Running.

5 License and Legal Information

5.1 Software License

McPherson Monochromator Control Software is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

McPherson Monochromator Control Software is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with McPherson Monochromator Control Software. If not, see `https://www.gnu.org/licenses/gpl-3.0.en.html`.

5.2 Open Source Credits

The McPherson Monochromator Control Software uses the following:

PyQt5, Copyright 2022 Riverbank Computing Limited, The Qt Company, under the GNU General Public License v3.0.

Qt5, Copyright 2023, The Qt Company, under the GNU General Public License v3.0.

5.3 Warranty and Liability

For information about warranty and liability, please refer to sections 15, 16, and 17 of the GNU Public License. The entire text of the relevant license is given in 'License.txt', the 'COPYING' file, and at `https://www.gnu.org/licenses/gpl-3.0.en.html`. For convenience, the relevant sections are shown below:

15. Disclaimer of Warranty.

THERE IS NO WARRANTY FOR THE PROGRAM, TO THE EXTENT PERMITTED BY APPLICABLE LAW. EXCEPT WHEN OTHERWISE STATED IN WRITING THE COPYRIGHT HOLDERS AND/OR OTHER PARTIES PROVIDE THE PROGRAM "AS IS" WITHOUT WARRANTY OF ANY KIND, EITHER EXPRESSED OR IMPLIED, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE. THE ENTIRE RISK AS TO THE QUALITY AND PERFORMANCE OF THE PROGRAM IS WITH YOU. SHOULD THE PROGRAM PROVE DEFECTIVE, YOU ASSUME THE COST OF ALL NECESSARY SERVICING, REPAIR OR CORRECTION.

16. Limitation of Liability.

IN NO EVENT UNLESS REQUIRED BY APPLICABLE LAW OR AGREED TO IN WRITING WILL ANY COPYRIGHT HOLDER, OR ANY OTHER PARTY WHO MODIFIES AND/OR

CONVEYS THE PROGRAM AS PERMITTED ABOVE, BE LIABLE TO YOU FOR DAMAGES, INCLUDING ANY GENERAL, SPECIAL, INCIDENTAL OR CONSEQUENTIAL DAMAGES ARISING OUT OF THE USE OR INABILITY TO USE THE PROGRAM (INCLUDING BUT NOT LIMITED TO LOSS OF DATA OR DATA BEING RENDERED INACCURATE OR LOSSES SUSTAINED BY YOU OR THIRD PARTIES OR A FAILURE OF THE PROGRAM TO OPERATE WITH ANY OTHER PROGRAMS), EVEN IF SUCH HOLDER OR OTHER PARTY HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES.

17. Interpretation of Sections 15 and 16.

If the disclaimer of warranty and limitation of liability provided above cannot be given local legal effect according to their terms, reviewing courts shall apply local law that most closely approximates an absolute waiver of all civil liability in connection with the Program, unless a warranty or assumption of liability accompanies a copy of the Program in return for a fee.

5.4   Important Notice Regarding Electronics

Electrical equipment can be hazardous if not handled properly. It is important to ensure that all electrical instruments are used with appropriate grounding on power lines, and that electrically powered components are not manipulated or touched unless they have been switched off and disconnected from the power source.

McPherson Inc. will not be held liable for any harm or damages caused by the equipment if the instructions contained in the respective manual(s) are not properly followed, or if the repairs are performed by personnel who are not trained or licensed by the company. It is the user's responsibility to follow all instructions and use the equipment in accordance with the manufacturer's guidelines.

6   About Us

6.1   McPherson

This software was designed for McPherson and is intended for use primarily with McPherson hardware. For information on McPherson, please visit `mcphersoninc.com`.

6.2   Contact Information

EMAIL: mcp@mcphersoninc.com
PHONE: (978) 256-4512, 1-800-255-1055

You can send an email to **mcp@mcphersoninc.com** and we will respond to you as soon as possible. If you prefer to speak with someone over the phone, you can call us at **(978) 256-4512** or **1-800-255-1055**.

7   How to Contribute

To see the most current rules on contributing to the project, please visit `github.com/mitbailey/MMC/wiki`. The information found on the wiki supersede any information listed within this manual. To view the Contributor's Guide please visit `mitbailey.github.io/MMC`.

7.1 Reporting Bugs

Prior to reporting any bugs or issues, it is imperative that it is reproducible. Please attempt to recreate the issue, documenting the steps necessary to cause it. All bugs and issues should then be reported using GitHub's issue tracking system at github.com/mcpherson-inc/MMC/issues. Please also export the software's configuration at the time of the issue and be sure to attach it to your issue post (if the issue is a start-up crash or occurs before entering into the main interface window, it is not necessary to include the current configuration). To open a new issue, click on the "New Issue" button and fill out the form using the following issue template and sample:

Issue Template

Title Which is Descriptive of the Issue

Software Version
"Ran from downloaded EXE," "Compiled from source code," or "Ran from source code."

List the following only if you compiled or ran from source code:
Python Version
Instructions on how it was compiled or run.

Operating System

(1) List the steps necessary to reproduce the issue you experienced.
Make sure to include what buttons were pressed, values of relevant spin-boxes and drop-downs. Include images if possible.

(2) What happened? Describe the issue.
Describe the issue itself, and what happened immediately afterwards.

(3) List any error messages that appeared.
Be sure to include the text and title of any errors which appeared.

(4) Additional Notes
Anything you think may help us solve this issue.

Issue Sample

> **Program Crashes After Pressing "Scan" Button**
>
> MMCS v1.1
> Ran from downloaded EXE.
>
> Windows 10
>
> (1) List the steps necessary to reproduce the issue you experienced.
> I first launched the program and successfully connected one Picoammeter and one 792. The main window opened and I configured the devices / axes in the Machine Configuration window (see attached config export file for value details). I then set the main axis scan to start: 100 nm, stop: 250 nm, step: 10 nm. I then pressed the "Scan" button.
>
> (2) What happened? Describe the issue.
> When I pressed "Scan" the program immediately crashed.
>
> (3) List any error messages that appeared.
> No error messages appeared.
>
> (4) Additional Notes
> N/A

7.2   Requesting Features

All feature requests should include justification including why this feature would help your specific use case and why it would help the community of program users.

To see the most current rules on contributing to the project, please visit github.com/mitbailey/MMC/wiki. To view the Contributor's Guide please visit mitbailey.github.io/MMC.

7.3   Contributing Code

To see the most current rules on contributing to the project, please visit github.com/mitbailey/MMC/wiki. To view the Contributor's Guide please visit mitbailey.github.io/MMC.