Computers, Software, and Scripting copy

Please see below the necessary software and installation instructions.

Connecting to the Laboratory Data Backup (OreBits)

All computers must be backed up routinely (at least once per week) to the group OreBits share. Please find below instructions for accessing/backing up data. Please feel free to update the document below with any relevant information:

OreBits_Info.docx

Note: You must enter your username as ADIT\username when connecting to OreBits!

Note: You may still retain backups to your Mines OneDrive if you so choose - HOWEVER: When you leave Mines, your OneDrive account gets deleted! To avoid data loss, please back up your research data at least once per week to the OreBits drive.

Connecting to the Lab Desktop and Laptop

Connect to the lab computer via TeamViewer to access the Gamry and TOPAS.

Desktop TeamViewer ID	502 366 908
Desktop Password	Argyrodite
Laptop TeamViewer ID	1 506 577 723
Laptop Password	FastLi+Ions

Software Installation

Python

Python is a powerful open-source coding language used extensively for data analysis and visualization. Python is used by our group, by beam lines, and in collaborations, so developing proficiency is a must.

Python Installation Instructions

Install **Python 3** via Anaconda. Put it in the suggested Directory. Use the instructions provided for your operating system. (Free Download | Anaconda)

Install **Jupyter Notebooks** (https://jupyter.org/install). Use `conda install -c conda-forge jupyterlab`. Once installed, you will be able to open Jupyter Notebook by typing `jupyter-notebook` in the terminal (in Mac). You can also start Jupyter Notebooks through Conda Navigator.

Other useful packages (can be installed/compiled) as necessary using the terminal/Conda command prompt:

- NumPy (`conda install numpy`)
- SciPy (`conda install scipy`)
- Matplotlib (`conda install matplotlib`)

Creating Multiple Python Environments (for advanced users)

While any *ad hoc* code you write should be written for Python 3, there are several legacy applications we use that may require Python 2.7, and thus it may be useful to have access to multiple versions of Python that you can switch between.

To create multiple Python environments that will be accessible in Jupyter Notebooks (written for MacOS):

In terminal, run:

```
conda install ipykernel
python -m ipykernel install --user --name <some-env> --display-name "<name-of-your-kernel>"
```

Resources:

- Switching between Python 2 and Python 3 environments — Anaconda documentation
- Enable multiple kernels in Jupyter Notebooks

To make nice fonts (Helvetica) for plots in Python, add these lines to the beginning of your code (after you import packages). This will also obey LaTex commands (i.e., ^{5} gives a superscripted "5"). FYI you will need to retype the single quotes in your Python Code!

```
from matplotlib.pyplot import rc
rc('text', usetex=True)
rc('font',**{'family':'sans-serif','sans-serif':['Helvetica']},size='14')
rc('text.latex',preamble=r'\usepackage{sfmath}')
```

SRC's Using TeX in Python Troubleshooting Guide

Tex_to_Python_Troubleshooting.pdf

How to get Helvetica to work on Windows:

- Download Helvetica.ttf (here)
- Make sure Tex works (see SRC guide above)
- Open Control Panel, search for Fonts, drag and drop Helvetica.ttf into Fonts window
- Restart Anaconda several times (i.e. close the entire program; restarting the kernel only will not work)
- Reopen Anaconda/Jupyter-Notebook and try again.
- If you had difficulties with LaTex stuff above, you will be prompted to install packages multiple times. Say okay to all of them.
- You may need to restart Anaconda one more time.

New to Python? Try this tutorial by Dr. Maughan!

Python_crash_course.zip

GitHub

GitHub is used to manage and update commonly-used code developed in the Maughan Lab. You may join the Maughan Lab GitHub here: Maughan-Lab

Current repositories:

- py_figures (Jupyter notebooks for making nice figures)
- faults (WIP)

Direct any questions about GitHub / repos to Sinclair

Grace

Xmgrace or Qtgrace is an open source 2D plotting software used to make high-quality scientific plots and figures. It also has some rudimentary data processing capabilities.

QtGrace For Windows and Mac

Download from SourceForge (QtGrace) and follow the installation instructions.

For Windows installation:

The actual application/icon will be located in ...\Program Files\Qtgrace\bin\. You can create a desktop shortcut.

The Default.agr template is located in ...\Program Files\Qtgrace\Templates\. Please replace the provided Default.agr with the file located in the "Grace Default Styles" subsection below, which will give you much better formatting and color selections.

Xmgrace

This is an old-school version of Grace for Unix systems that runs just slightly differently from Qtgrace. I like it because it's familiar to me, but Qtgrace has the same (and in some cases, better) functionality, so either version is fine.

Download instructions for Xmgrace for Mac:

First, download Xquartz (XQuartz). **IMPORTANT!** You must download an older version (version 2.7.9) - Newer versions do not work!

Log out of your computer login (you may want to just restart your computer).

Check that Xquartz is working properly. Open a terminal and type `xeyes`. A set of eyes should appear on your desktop if Xquartz is working properly.

Install Homebrew by running the following command in the terminal:

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

Run this command in the terminal: `echo '--disable-epsv' >> ~/.curlrc`

Now, run this series of commands in the terminal:

```
brew update
brew doctor
brew upgrade
brew tap homebrew/x11
brew install grace
```

Xmgrace should now open when you type `xmgrace` in the terminal. You may need to restart your terminal or your computer.

These installation instructions were adapted from:
https://nokyotsu.com/qscripts/2011/05/installing-xmgrace-on-snow-lepoard.html

Grace Default Styles

In the Maughan lab, we use a different Default style than what is provided with the Xmgrace/Qtgrace installation.

The **Default.agr** file tells Grace what the default settings should be. On Mac/Linux, this file lives high up in the OS directories. It may live in either: "/usr/local/opt/grace/templates" or "/opt/local/lib/grace/templates". To update, replace the Default.agr with this file. You will need to do this in the terminal and have Administrator privileges.

Default.agr

If successful, opening Grace will give you a square graph window with the Helvetica typeface and a larger palette of colors. You may also add your own colors by opening the Default.agr in a text editor and adding colors.

In QtGrace, I believe there is a way within the GUI to set the pathname to the Default.agr.

Other Grace Resources

- Huge compilation of Grace symbol/character codes (Dallas R. Trinkle | MatSE at the University of Illinois | group:res_grace)
- Louic's WebBlog (http://blog.louic.nl/?p=249)
- Grace ASCII Character Codes (http://blog.louic.nl/files/ascii.html)
- Tips for Xmgrace (Tips for Xmgrace - LPTMS Wiki)

Here is an incomplete list of useful symbols and corresponding codes (more can be found in the ASCII Table above). Please add any more that you find useful!

Desired Symbol	Code
Subscripted "Z"	\sZ\N
Superscripted "Z"	\SZ\N
Italics "Z"	\qZ\Q
Uppercase Greek (example: Omega) (w=omega, q = theta, l = lambda, a = alpha, etc.)	\xW\f{}
Lowercase Greek (example: omega) (w=omega, q = theta, l = lambda, a = alpha, etc.)	\xw\f{}
Celcius (°)	\c0\C
Angstrom (Å)	\cA\C
m-dash (–)	\x-\f{}
Overbar "3"	\o3\O

GSAS-II

GSAS stands for General Structure Analysis System, and is developed at the Advanced Photon Source, Argonne National Laboratory. GSAS-II is open-source software for the analysis of X-ray and neutron scattering data. In the Maughan lab, most structural analysis will be performed using TOPAS, but GSASII is used to supplement this software as a free tool for structural analysis that can be used on personal computers.

Follow the installation instructions for your OS here: GSAS-II - Crystallography Data Analysis Software

TOPAS v6

TOPAS is an extremely powerful structural analysis program for analysis of X-ray and neutron scattering data. The Maughan group has 3 license keys to be shared among all members. The chemistry department also has access to shared licenses available for borrowing/checkout.

TOPAS Resources

TOPAS Wiki

TOPAS 6 Technical Reference.pdf

TOPAS 6 Tutorial.pdf

TOPAS 6 Users Manual.pdf

TOPAS 6 Whats New.pdf

Chemistry D2 Phaser

Instrument Parameter file for TOPAS refinements: CH_Bruker_Jun2022_FINAL.par

11-BM-B

Instrument Parameter file for TOPAS refinements: 11BM_inst.par

Note that you will need to change the wavelength to the calibrated wavelength from your experiment under "Emission Profile"

VESTA

VESTA is an open-source software for visualizing crystal structures (VESTA).

Avogadro

Avogadro is an open-source software for visualizing molecular structures (Avogadro - Free cross-platform molecular editor).

LaTex

LaTex is a high-quality typesetting system for preparing documents. We will heavily use LaTex for writing and editing manuscripts, longer scientific documents (i.e., theses/dissertations), or even CVs and Resumes. (LaTeX - A document preparation system)

Please install the LaTex distribution for your operating system (Get LaTeX - Mac OS, Windows, Linux)

Overleaf

Overleaf is an online LaTex editor that is user-friendly and useful for collaborations/edits. Single-user accounts are free to use; the Maughan lab owns a yearly subscription, which enables tracked changes and other extra functionalities.

LaTexIt

LaTexIt is a useful little tool to write equations and mathematical expressions to include in presentations. Get it here: https://www.chachatelier.fr/latexit/latexit-downloads.php?lang=en

DeTexify

DeTexify is an applet that converts handwritten symbols to LaTex code. Very useful for symbols you don't recognize.

Useful LaTex Symbols and Codes

Table 2.2: Accents and Special Characters.

ò	\‘o	ó	\’o	ô	\^o	õ	\~o
ō	\=o	ȯ	\.o	ö	\"o	ç	\c c
ǒ	\u o	ǒ	\v o	ő	\H o	ǫ	\c o
ọ	\d o	o͟	\b o	o͡o	\t oo		
œ	\oe	Œ	\OE	æ	\ae	Æ	\AE
å	\aa	Å	\AA				
ø	\o	Ø	\O	ł	\l	Ł	\L
ı	\i	ȷ	\j	¡	!‘	¿	?‘

Generate LaTex tables

Useful tool for visually creating tables and converting them to LaTex code - Create LaTeX tables online – TablesGenerator.com

Cross Reference Multiple .tex files in Overleaf

This is super helpful if you have a main text document and supplemental info and want to reference figures from the SI in your main text!

Cross referencing with the xr package in Overleaf -...

Citation Management Software

Find a citation management software that works for you, but it *must* interface with LaTex/BibTex and ideally would also interface with Microsoft Word. I use Mendeley, but Zotero, Jabref, or Bibdesk are fine options as well.

Hot tip! I would *highly* recommend starting early using citation management software. When you add new citations, make sure that the information is correct (i.e. journal abbreviation, volume, pages, etc.). If a function exists to organize your references in the application, use it. Having a well-curated library of references will save you a lot of time when you are writing papers or thesis/dissertation!

Text Editor

I like BBedit, but find one that works best for you!

Other Options:

- NOTEPAD++ (Windows)
- Bluefish Editor (Mac, Linux)
- TextWrangler (Mac)
- Smultron (Mac)
- Caditor (Windows)
- gedit (Linux)
- GNU Emacs (Windows, Mac, Linux)
- Crimson Editor (Windows)

Gnu Image Manipulation Program (GIMP)

GIMP is an open-source version of Photoshop. (GIMP)

Terminal/Command Line, Scripting

Computer literacy is necessary to succeed in science. Scripting can be used to automate tedious tasks or streamline data processing. This section is intended as a "Quick Start Guide" for navigating the terminal on Unix-based systems.

A Word of Warning: The terminal can give you access to files that are critical for your computer/operating system to run properly! Be extremely conscientious when executing commands that manipulate files/commands higher up in the OS directories. If you are unsure, I (Annalise) am happy to assist you!

General Terminal Use

Linux_Guide.pdf

Creating aliases with the .bashrc (for Mac/Linux)

Similarly to how `cd` and `ls` are commands that the terminal recognizes that do specific actions, you can create your own commands through the use of an *alias*. These aliases are saved in a hidden file called the .bashrc.

Example: Alias to open VESTA from the terminal

Opening the terminal and running `open -a VESTA` will open the VESTA program. But no one wants to type that every time! So we create a simpler command (alias):

To create the VESTA alias:

Open the .bashrc in a text editor (usually located in ~/.bashrc).

Add: `alias vesta='open -a VESTA'` to the .bashrc file and save it.

Restart the terminal and your alias should work! (**Note:** If you don't restart the terminal, it has no way of knowing that you changed the .bashrc. See the Special note for Macs below).

Now, typing `vesta` in the terminal will open VESTA.

Special note for Macs

While the aliases are stored in ~/.bashrc, the Mac terminal sources ~/.bash_profile when it opens. For your aliases to work, open ~/.bash_profile and add the line `source ~/.bashrc` to the end. Then save and reopen your terminal.

Gamry Framework

Gamry_Library.pdf