Getting Started

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Preface

This is a Quarto book.

To learn more about Quarto books visit https://quarto.org/docs/books.

```
1 + 1
```

```
[1] 2
```

1 Introduction

This is a book created from markdown and executable code.

See Knuth (1984) for additional discussion of literate programming.

```
1 + 1
```

```
[1] 2
```

2 Summary

In summary, this book has no content whatsoever.

```
1 + 1
```

```
[1] 2
```

3 Software Needed

3.1 R and RStudio

Go to RStudio Desktop download page to download the R and RStudio Desktop installers.

> **Note**
>
> You need to install R first, then RStudio.

The R link will take you to the The Comprehensive R Archive Network where you can download an R installer for your operating system.

The RStudio link will download the apropriate installer for your operating system.

Download and launch the installers and follow the installation instructions.

3.2 Git and a GitHub Account

Git and GitHub

> **Tip**
>
> We will use `git` within RStudio. On macOS, RStudio with echo the mac terminal. I am using Oh My Zsh as my `zsh` framework, and iTerm2 as my terminal emulator rather than the macOS default terminal application. I also have the latest `git` version installed through Homebrew.
> This means that I need to adjust the settings in RStudio to use my `zsh` environment. Go to *Tools* → *Global Options* → *Terminal* and choose `Zsh` from the drop-down menu for the *New terminals open with* option.

3.3 VS Code

Download and launch the installer and follow the instructions.

Visual Studio Code

3.4 Zotero

3.4.1 Zotero Desktop

Zotero is available for macOS, Windows, Linux, and iOS.

Download Zotero from the Zotero website.

Installation is straightforward, but installation instructions are available if needed.

3.4.2 Zotero Connector

Also install the Zotero Connector for the Chrome web browser for easy importing of items into your Zotero library.

3.4.3 Better BibTeX for Zotero

To easily cite references in your Quarto documents in RStudio, install the Better BibTeX plugin.

3.4.4 Zotero 7 Beta

There is a beta release for Zotero 7. This has (I believe) a nicer interface, and new features. See the Zotero 7 beta announcement for more information.

3.5 ChimeraX

1. Go to the ChimeraX download page.
2. Download the installer appropriate for your operating system.
3. Accept the license agreement.
4. Follow the instructions for your operating system. For example, on macOS (M2 chip):
5. Open the disk image.
6. Drag the ChimeraX application to your Applications folder.

3.6 RealVNC Viewer

3.6.1 RealVNC Viewer

To connect to NMRbox to run GROMACS simulations, you need to install VNC software. VNC is an abbreviation of Virtual Network Computing, which is another way to say screen sharing. NMRbox uses RealVNC Server to which we can connect using the client software, RealVNC Viewer.

Download and install the software following the onscreen instructions (for macOS, drag the app to the *Applications* folder).

3.6.1.1 Troubleshooting

copy and paste to NMRbox stops working In Terminal on NMRbox, type the following: `vncconfig &` and hit return. See How to fix VNC Viewer copy-paste not working for additional help.

3.7 Optional Software

3.7.1 Anaconda

3.7.1.1 Update Homebrew

In terminal:

```
cd ~
brew update                                                    ①
brew upgrade                                                   ②
```

① Update the Homebrew package manager.
② Upgrade the packages in Homebrew. *Note*: This can take a long time (hours) depending on how many packages need upgrading.

3.7.1.2 Install Anaconda

```
brew install --cask anaconda
```

After installation is complete, add the path to `.zshrc` and restart shell.

```
echo 'export PATH="/usr/local/Homebrew/anaconda3/bin:$PATH"' >> ~/.zshrc
source ~/.zshrc
```

3.7.1.3 Activate Anaconda

```
source /usr/local/Homebrew/anaconda3/bin/activate                    ①
conda init zsh                                                       ②
```

① Use the path to the Homebrew-installed Anaconda.
② Initialize your preferred shell to work with `conda`.

Test the installation.

```
conda --version
conda 25.4.0
```

Success!

3.7.1.4 Create and activate a `conda` Environment for the Plumed Masterclass Tutuorial

```
conda create --name plumed-masterclass-2022
```

Activate the environment with:

```
conda activate plumed-masterclass-2022
```

> **Note**
>
> To deactivate an active environment, use
>
> ```
> conda deactivate
> ```

4 Scratch Pad

Just a place for quick notes

References

Knuth, Donald E. 1984. “Literate Programming.” *Comput. J.* 27 (2): 97–111. https://doi.org/10.1093/comjnl/27.2.97.