Stellar Spectroscopy Workshop software requirements

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Contents

About

This document provides a list of software requirements and installation procedures for the Stellar Spectroscopy Workshop at the University of Tartu, Estonia from 27-28th September 2023. You will need a Mac or a Linux(Ubuntu) operating system on your computer. You can also use/install a virtual environment of Linux if you have Windows. We will have a separate Python environment for the software so that installing different modules doesn't affect the general functioning of your computer. We will use the terminal to install most software.

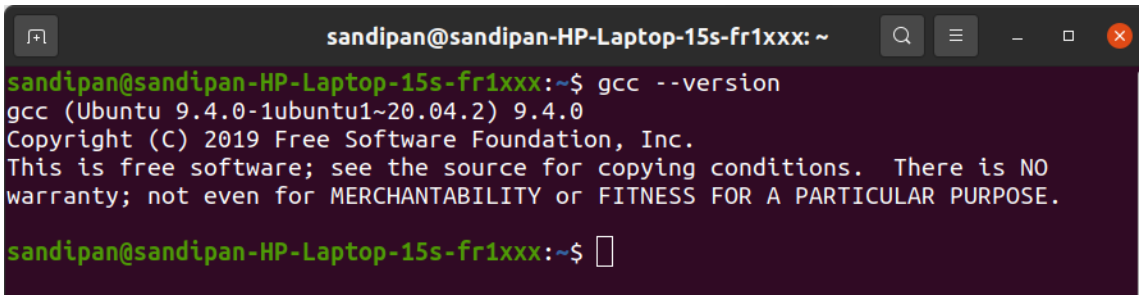
The commands for installation are shown in the boxes. Some boxes have multiple commands, run them one by one. You can also directly copy and paste the commands from this pdf. You will see the expected outputs in the figures of the terminal windows beneath each command. The versions of packages installed can be different from the ones shown in the picture. Do not panic, that should not cause any issues.

Instructions for Ubuntu

2.0.1 gcc, gfortran and libgfortran5

Check if gcc exists with the following command in your terminal-

```
gcc --version
```

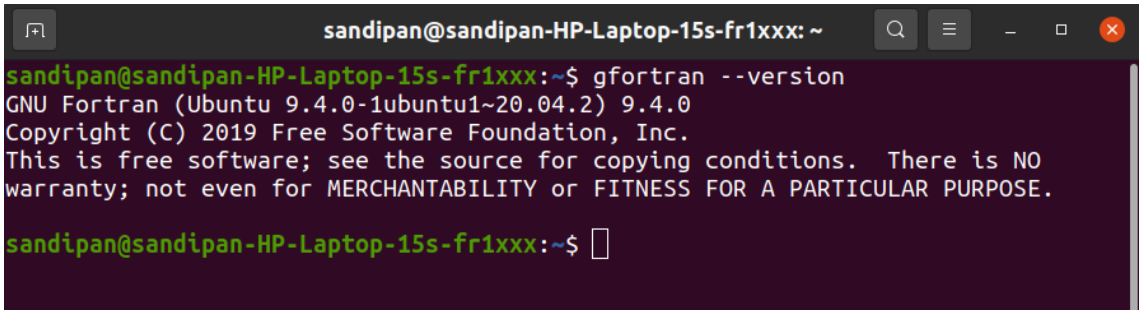


If not, install it with the following command -

```
sudo apt-get install build-essential
```

Check if gfortran exists with the following command in your command prompt/terminal-

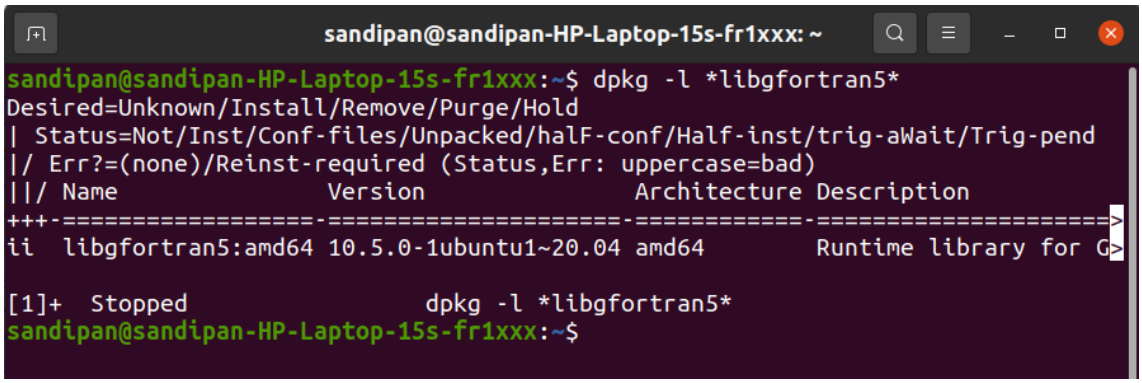
```
gfortran --version
```



If not, install it with the following command -

```
sudo apt-get update
sudo apt-get install gfortran
```

Check if libgfortran5 exists with the following command in your command prompt/terminal-




```
dpkg -l *libgfortran5*
```

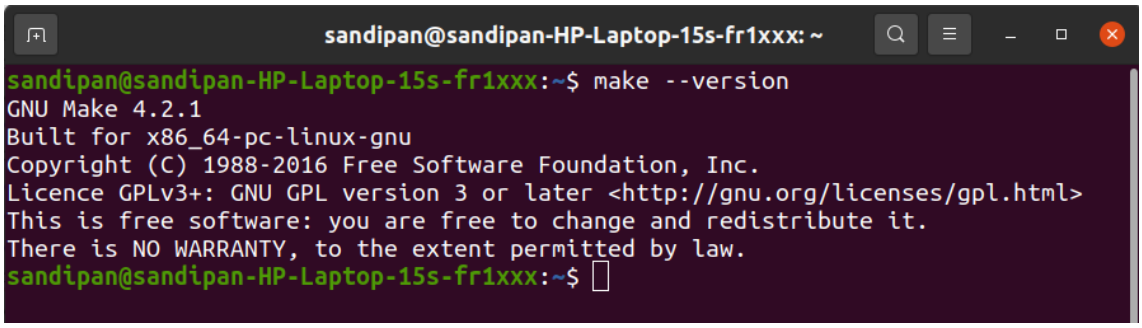
If not, install it with the following command -

```
sudo apt-get update
sudo apt-get install libgfortran5
```

2.0.2 make

Check if make exists with the following command in your command prompt/terminal-

```
make --version
```



If not, install it with the following command -

```
sudo apt-get update
sudo apt-get install make
```

2.0.3 Python3

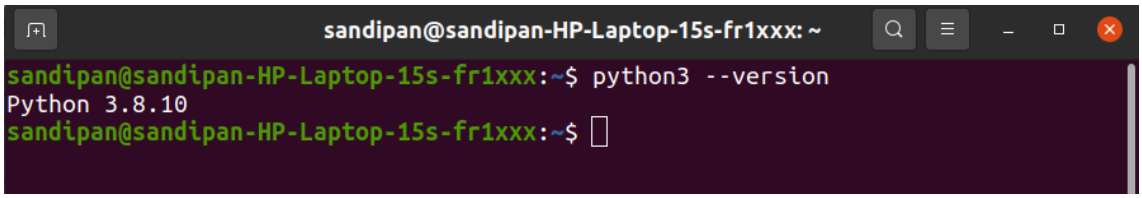
Check if Python3 exists with the following command in your command prompt/terminal-

```
python3 --version
```

If not, install it with the following command -

```
sudo apt-get update
sudo apt-get install python3
```

You can also install specific versions of Python3. We have tested it with Python 3.8 and above and it works.



2.0.4 pip3

Check if Python3 exists with the following command in your command prompt/terminal-

```
pip3 --version
```

If not, install it with the following command -

```
sudo apt install python3-pip
```

2.0.5 Setting up Python3 environment

Create the Python environment and all its necessary modules with the following command in your command prompt/terminal-

```
sudo apt-get update
sudo apt install python3-venv
mkdir ~/specwrk-python
cd ~/specwrk-python
python3 -m venv spectroscopy-workshop
source spectroscopy-workshop/bin/activate
pip3 install wheel
pip3 install matplotlib plotly ipywidgets pysme-astro
```

Note - Users having Anaconda installed can instead make a conda environment. In case you want to setup the environment following the above steps, deactivate your current anaconda environment for installation and every time, you open a new terminal to run ZEEMAN or pySME. Run the following command in your command prompt/terminal to deactivate the anaconda environment -

```
conda deactivate
```

Note - Whenever you open a new terminal next time to use ZEEMAN or pySME, you need to activate spectroscopy-workshop python environment by running the following command in your command prompt/terminal -

```
source ~/specwrk-python/spectroscopy-workshop/bin/activate
```

2.0.6 ZEEMAN

To download ZEEMAN either click on the link below or you can install it from your terminal.

https://owncloud.ut.ee/owncloud/s/zq8M6i8fyRoqHjf

To install it from your terminal navigate to the folder where you want to install ZEEMAN using terminal, and then run the following command in your command prompt/terminal -

```
wget https://owncloud.ut.ee/owncloud/s/zq8M6i8fyRoqHjf/download/ZEEMAN.tar.gz
```

Extract the ZEEMAN.tar.gz file. You can extract the file from the command prompt/terminal by first navigating to the folder where your ZEEMAN.tar.gz file is through your terminal and run the following command -

```
tar -zxvf ZEEMAN.tar.gz
```

Using the terminal, navigate to the ZEEMAN folder where there is a Makefile and run the following commands -

```
make zuc
make lma
```

2.0.7 pySME

pySME is installed when you set up the Python environment. You can test if it works by first downloading these files either from the link below or through your terminal -

https://owncloud.ut.ee/owncloud/s/SdR7E9CJdj4Lf6N

To install it from your terminal navigate to the folder where you want to install the test files using terminal, and then run the following command in your command prompt/terminal -

```
wget https://owncloud.ut.ee/owncloud/s/SdR7E9CJdj4Lf6N/download/smetest.tar.gz
```

Extract the folder and navigate into it through the terminal. You can then run the following command to test pySME -

```
python3 minimum.py
```

If you get an error on missing dependencies, you can install them by running -

```
pip3 install [module name]
```

Instructions for Mac

3.0.1 Hombrew Install

Check if homebrew exists with the following command in your terminal-

```
brew --version
```

```
kertumetsoja@Kertus-MacBook-Pro ~ % brew --version
Homebrew 4.1.11
Homebrew/homebrew-core (git revision fe20814d11c; last commit 2023-09-12)
kertumetsoja@Kertus-MacBook-Pro ~ %
```

If not, install it from Homebrew page (click here) with the first command.

3.0.2 gcc, gfortran and libgfortran5

Check if gcc exists with the following command in your terminal-

```
brew info gcc
```

```
kertumetsoja@Kertus-MacBook-Pro ~ % brew info gcc
==> gcc: stable 13.2.0 (bottled), HEAD
GNU compiler collection
https://gcc.gnu.org/
/usr/local/Cellar/gcc/13.2.0 (1,590 files, 421.8MB) *
  Poured from bottle using the formulae.brew.sh API on 2023-09-19 at 16:30:56
From: https://github.com/Homebrew/homebrew-core/blob/HEAD/Formula/g/gcc.rb
License: GPL-3.0-or-later with GCC-exception-3.1
==> Dependencies
Required: gmp ✔, isl ✔, libmpc ✔, mpfr ✔, zstd ✔
==> Options
--HEAD
        Install HEAD version
==> Analytics
install: 124,144 (30 days), 291,090 (90 days), 583,232 (365 days)
install-on-request: 61,403 (30 days), 142,965 (90 days), 293,549 (365 days)
build-error: 95 (30 days)
kertumetsoja@Kertus-MacBook-Pro ~ %
```

If not, install it with the following command -

```
brew install gcc
```

Installing gcc should also install gfortran. You can check if gfortran exists with the following command in your command prompt/terminal -

```
gfortran --version
```

```
kertumetsoja@Kertus-MBP ~ % gfortran --version
GNU Fortran (Homebrew GCC 13.2.0) 13.2.0
Copyright (C) 2023 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.

kertumetsoja@Kertus-MBP ~ %
```

3.0.3 make

Check if make exists with the following command in your command prompt/terminal-

```
make --version
```

```
kertumetsoja@Kertus-MacBook-Pro ~ % make --version
GNU Make 3.81
Copyright (C) 2006  Free Software Foundation, Inc.
This is free software; see the source for copying conditions.
There is NO warranty; not even for MERCHANTABILITY or FITNESS FOR A
PARTICULAR PURPOSE.

This program built for i386-apple-darwin11.3.0
kertumetsoja@Kertus-MacBook-Pro ~ %
```

If not, install it with the following command -

```
brew install make
```

3.0.4 Python3

Check if Python3 exists with the following command in your command prompt/terminal-

```
python3 --version
```

```
kertumetsoja@Kertus-MacBook-Pro ~ % python3 --version
Python 3.10.7
kertumetsoja@Kertus-MacBook-Pro ~ %
```

If not, install it with the following command -

```
brew install python3
```

You can also install specific versions of Python3. We have tested it with Python 3.8 and above and it works.

3.0.5 pip3

Check if pip3 exists with the following command in your command prompt/terminal-

```
pip3 --version
```

If you have Python3 installed, pip3 should exist too. Otherwise, install Python3 as mentioned in the previous section.

```
kertumetsoja@Kertus-MacBook-Pro ~ % pip3 --version
pip 23.2.1 from /Library/Frameworks/Python.framework/Versions/3.10/lib/python3.1
0/site-packages/pip (python 3.10)
kertumetsoja@Kertus-MacBook-Pro ~ %
```

3.0.6 Setting up Python3 environment

Create the Python environment and all its necessary modules with the following command in your command prompt/terminal-

```
brew install virtualenv
mkdir ~/specwrk-python
cd ~/specwrk-python
virtualenv -p python3 spectroscopy-workshop
source spectroscopy-workshop/bin/activate
pip3 install wheel
pip3 install matplotlib plotly ipywidgets pysme-astro
```

Note - We installed pip3 instead of brew in the last command because astropy package is not available in brew.

Note - Users having Anaconda installed can make a conda environment instead. In case you want to setup the environment following the above steps, deactivate your current anaconda environment for installation and every time, you open a new terminal to run ZEEMAN or pySME. Run the following command in your command prompt/terminal to deactivate the anaconda environment -

```
conda deactivate
```

Note - Whenever you open a new terminal next time to use ZEEMAN or pySME, you need to activate spectroscopy-workshop python environment by running the following command in your command prompt/terminal -

```
source ~/specwrk-python/spectroscopy-workshop/bin/activate
```

3.0.7 ZEEMAN

To download ZEEMAN either click on the link below or you can install it from your terminal.

https://owncloud.ut.ee/owncloud/s/zq8M6i8fyRoqHjf

To install it from your terminal navigate to the folder where you want to install ZEEMAN using terminal, and then run the following command in your command prompt/terminal -

```
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```

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```
tar -zxvf ZEEMAN.tar.gz
```

Using the terminal, navigate to the ZEEMAN folder where there is a Makefile and run the following commands -

```
make zuc
make lma
```

3.0.8 pySME

pySME is installed when you set up the Python environment. You can test if it works by first downloading these files either from the link below or through your terminal -

https://owncloud.ut.ee/owncloud/s/SdR7E9CJdj4Lf6N

To install it from your terminal navigate to the folder where you want to install the test files using terminal, and then run the following command in your command prompt/terminal -

```
wget https://owncloud.ut.ee/owncloud/s/SdR7E9CJdj4Lf6N/download/smetest.tar.gz
```

Extract the folder and navigate into it through the terminal. You can then run the following command to test pySME -

```
python3 minimum.py
```

If you get an error on missing dependencies, you can install them by running -

```
pip3 install [module name]
```

Note - If you have the error mentioned in the next page, you have to run the following command every time you open a new terminal(and activate the spectroscopy-workshop environment) for using pySME -

```
export DYLD_LIBRARY_PATH=$DYLD_LIBRARY_PATH:/usr/local/gfortran/lib
```

This is a makeshift solution, but you can look for ways to add this path permanently to the bashrc/source files, but we haven't tried that.

```
(spectroscopy-workshop) kertumetsoja@Kertus-MBP specwrk-python % python3 minimum
.py
/Users/kertumetsoja/specwrk-python/spectroscopy-workshop/lib/python3.11/site-pac
kages/pysme/smelib/setup.py:5: DeprecationWarning:

  `numpy.distutils` is deprecated since NumPy 1.23.0, as a result
  of the deprecation of `distutils` itself. It will be removed for
  Python >= 3.12. For older Python versions it will remain present.
  It is recommended to use `setuptools < 60.0` for those Python versions.
  For more details, see:
    https://numpy.org/devdocs/reference/distutils_status_migration.html


  import numpy.distutils.misc_util
running build_ext
Traceback (most recent call last):
  File "/Users/kertumetsoja/specwrk-python/minimum.py", line 11, in <module>
    from pysme import sme as SME
  File "/Users/kertumetsoja/specwrk-python/spectroscopy-workshop/lib/python3.11/
site-packages/pysme/sme.py", line 19, in <module>
    from .linelist.linelist import LineList
  File "/Users/kertumetsoja/specwrk-python/spectroscopy-workshop/lib/python3.11/
site-packages/pysme/linelist/linelist.py", line 18, in <module>
    from ..util import air2vac, vac2air
  File "/Users/kertumetsoja/specwrk-python/spectroscopy-workshop/lib/python3.11/
site-packages/pysme/util.py", line 25, in <module>
    from .sme_synth import SME_DLL
  File "/Users/kertumetsoja/specwrk-python/spectroscopy-workshop/lib/python3.11/
site-packages/pysme/sme_synth.py", line 19, in <module>
    cdll.LoadLibrary(libfile)
  File "/usr/local/Cellar/python@3.11/3.11.5/Frameworks/Python.framework/Version
s/3.11/lib/python3.11/ctypes/__init__.py", line 454, in LoadLibrary
    return self._dlltype(name)
           ^^^^^^^^^^^^^^^^^^^
  File "/usr/local/Cellar/python@3.11/3.11.5/Frameworks/Python.framework/Version
s/3.11/lib/python3.11/ctypes/__init__.py", line 376, in __init__
    self._handle = _dlopen(self._name, mode)
                   ^^^^^^^^^^^^^^^^^^^^^^^^^
OSError: dlopen(/Users/kertumetsoja/specwrk-python/spectroscopy-workshop/lib/pyt
hon3.11/site-packages/pysme/lib/libsme.dylib, 0x0006): Library not loaded: /usr/
local/opt/gcc@9/lib/gcc/9/libgfortran.5.dylib
  Referenced from: <B97AF636-A2AE-34E7-BFF7-76FABAEC42B3> /Users/kertumetsoja/sp
ecwrk-python/spectroscopy-workshop/lib/python3.11/site-packages/pysme/lib/libsme
.dylib
  Reason: tried: '/usr/local/opt/gcc@9/lib/gcc/9/libgfortran.5.dylib' (no such f
ile), '/System/Volumes/Preboot/Cryptexes/OS/usr/local/opt/gcc@9/lib/gcc/9/libgfo
rtran.5.dylib' (no such file), '/usr/local/opt/gcc@9/lib/gcc/9/libgfortran.5.dyl
ib' (no such file), '/usr/local/lib/libgfortran.5.dylib' (no such file), '/usr/l
ib/libgfortran.5.dylib' (no such file, not in dyld cache)
(spectroscopy-workshop) kertumetsoja@Kertus-MBP specwrk-python %
```