Installing and using 3D-PDR for the Hel.A.S. Summer School 2022

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3D-PDR is a combined FORTRAN 90/95 and C++ OpenMP code. You will therefore need FORTRAN and C compilers. The plotting tool is in Python. To install the code, you will first need to install the SUNDIALS package. Please follow the next steps.

Step 1: Untar the `3DPDR_HelAS.tgz` file

As a first step, you may untar the `3DPDR_HelAS.tgz` file in any directory you would like to (e.g. your home ∼/). Simply type:

```
tar xvzf 3DPDR_HelAS.tgz
```

This will create the ∼`/3DPDR/` directory in which all files will be extracted.

Step 2: Install the SUNDIALS package

To install SUNDIALS, go to the directory:

```
~/3DPDR/src/sundials-2.5.0/
```

Now, type (in one continuous line):

```
./configure CC=gcc F77=gfortran --with-cflags="-fopenmp"
      --with-ldflags="-fopenmp" --with-fflags="-fopenmp"
      --prefix="ABSOLUTE-HOME-PATH/3DPDR/sundials"
```

Make sure at the end you type `sundials` and **not** the above path. This will automatically create a new directory called `sundials`. For example for the `--prefix` flag in my laptop, I type:

```
/home/tbisbas/data/Codes/3DPDR/sundials
```

After the above configuration is done and while still in ∼`/3DPDR/src/sundials-2.5.0/`, type

```
make
```

and then

```
make install
```

This will proceed with installing SUNDIALS in the directory specified in the `--prefix` flag. This directory will be needed in the `makefile` of 3D-PDR (see next step). Once you have successfully installed SUNDIALS, you will be able to proceed in installing 3D-PDR. Failure to install SUNDIALS will make impossible to proceed any further. Please refer to the `INSTALL_NOTES` file found in ∼`/3DPDR/src/sundials-2.5.0/` for full description of the installation process and additional help.

Step 3: Install the 3D-PDR code

You can now proceed with installing the main code. To do this, go to the directory ∼/3DPDR/src/ and edit the makefile. In the lines 8 and 9, the variables INCLUDES and LIBRARIES must be edited; replace the ABSOLUTE-HOME-PATH with the full directory to 3DPDR/. For example, in my laptop I have:

```
-I/home/tbisbas/data/Codes/3DPDR/sundials/include
-L/home/tbisbas/data/Codes/3DPDR/sundials/lib
```

Make sure to keep the -I and -L flags! After the above edit, you are ready to go! Type

```
make
```

while in the ∼/3DPDR/src/ directory. This will make the code and will automatically move the executable file to ∼/3DPDR/. Once this is done, you will need to test if the code is running fine.

Step 4: Test the code

To test if the code is running fine, in the directory ∼/3DPDR/ type

```
./3DPDR
```

and the code should start. Depending on your machine, it may take from $\sim 20 - 30$ seconds to a few minutes. Once the code is finished, in the directory ∼/3DPDR/sims/ several outputs will be written with the prefix test. To plot the outputs, go to ∼/3DPDR/plots/ and type

```
python test_plot.py
```

The following diagrams should appear on screen. If so, congratulations! You are ready for the hands-on exercises. For any question, please contact me. For the analysis, I will provide extra python scripts on the day of the exercise.

******In the case you won't be able to install the code, I will provide you with all the outputs to do the exercises******

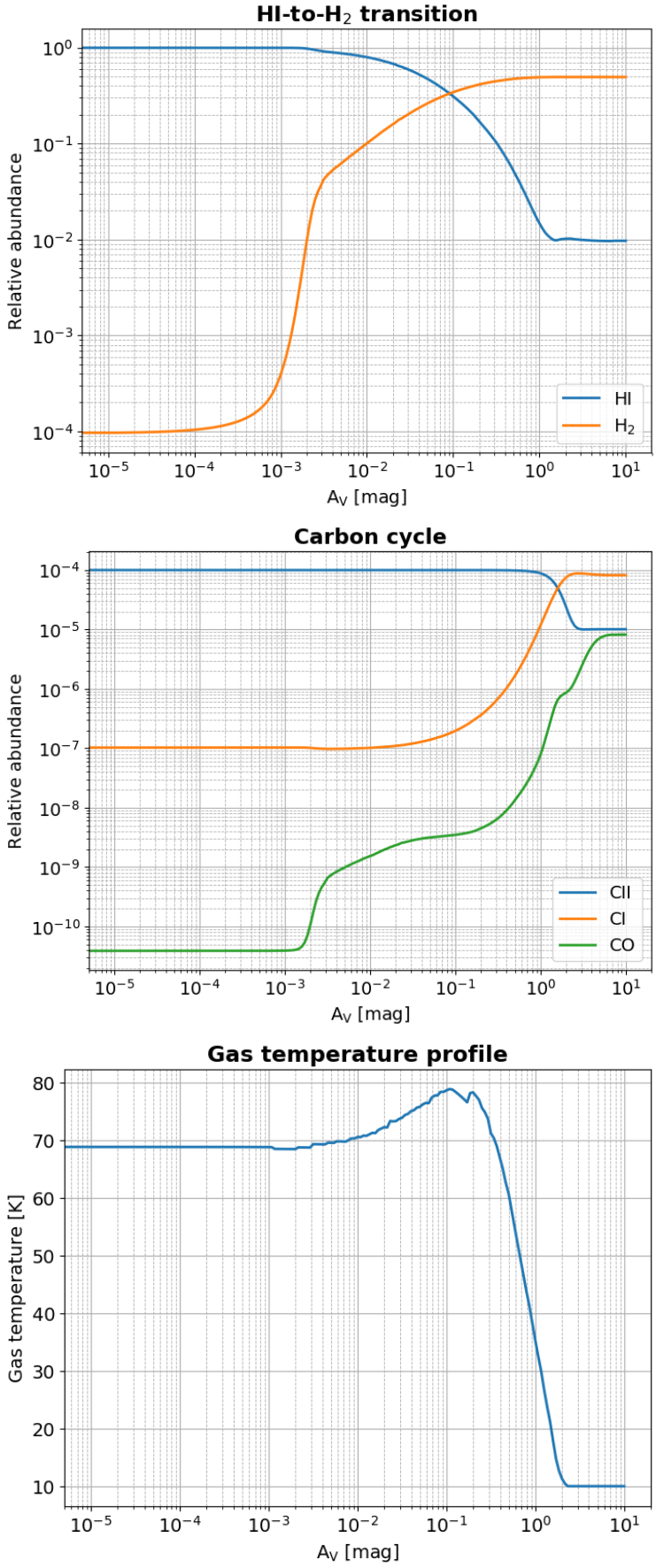

Figure 1: The outputs you should see after running 3D-PDR successfully