

# Driving Scientific Computations with Make

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# Notation used in this presentation

## Shell commands

Commands in the command line are prefixed with \$, e.g.

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## Placeholders

Placeholders for files or variables will be surrounded by [], e.g.

```
$ cat [A FILE] > [ANOTHER FILE]
```

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- Pretty much available in any modern Linux distributions as `GNU Make`.
- Full manual <https://www.gnu.org/software/make/manual/make.html>



# How does it work?

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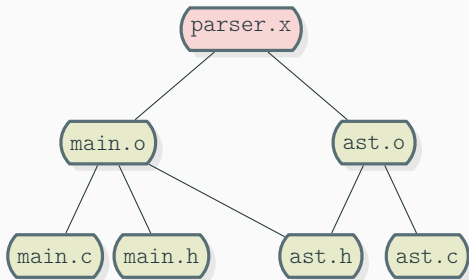
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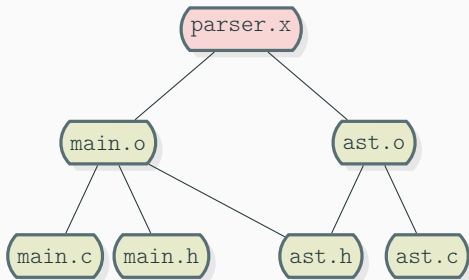
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**Figure 1:** Example file dependency graph

**In general, any set of files and rules works!**

# A Makefile Example

```
# Comments start with # as in bash
# Usually, one begins a file by setting some variables.
# For example:
COMPILER := gcc
LINKER := gcc

# The body of the Makefile consists of a set of rules
# which follow the following syntax:

# [TARGET] ... : [PREREQUISITES] ...
#     [RECIPE]

parser.x: main.o ast.o
    $(LINKER) main.o ast.o

main.o: main.h main.c ast.h
    $(COMPILER) -c main.c

ast.o: ast.h ast.c
    $(COMPILER) -c ast.o
```

# Decomposing a Rule Entry

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## Note

- `[RECIPE]` lines must be prefixed by a tab character
- Multiple `[RECIPE]` lines are allowed, but they are sent to different shells if not terminated by a backslash.

# Make Execution

Once a `Makefile` is written, `make` can be executed in a shell, in the same directory as the `Makefile`

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## Tip

One can select a particular `[TARGET]` to execute by passing it to `make`, as so

```
$ make [TARGET]
```

1

# Make basic features

Make is loaded with a bunch of functions. For example, one can load paths from the file-system,

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and much more, including conditionals and loops

[https://www.gnu.org/software/make/manual/html\\_node/Functions.html](https://www.gnu.org/software/make/manual/html_node/Functions.html).

# Make basic features

`Make` also generates a set of automatic variables that help in writing rules. For example, one can load the name of the target and prerequisites

```
requisites.txt: A couple of words
    echo $^ > $@

A couple of words:
```

1  
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where `$^` holds all prerequisites and `$@`, the target.

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where `$^` holds all prerequisites and `$@`, the target.

One can also write rules based on patterns, as so,

```
%.o: %.c
    gcc -c $< -o $@
```

1  
2

which allows for writing generic recipes a file type. In this case `$<` holds the name of the first prerequisite.

[https://www.gnu.org/software/make/manual/html\\_node/Automatic-Variables.html](https://www.gnu.org/software/make/manual/html_node/Automatic-Variables.html)

[https://www.gnu.org/software/make/manual/html\\_node/Pattern-Intro.html](https://www.gnu.org/software/make/manual/html_node/Pattern-Intro.html)

## PHONY targets

Sometimes it is useful to write rules which are not associated with a file. For example,

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clean:
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Normally, this rule will try to find a file named `clean` in the working directory, and if it exists the rule would not be executed. To let `Make` know this is a dummy rule one can use the `.PHONY` declaration:

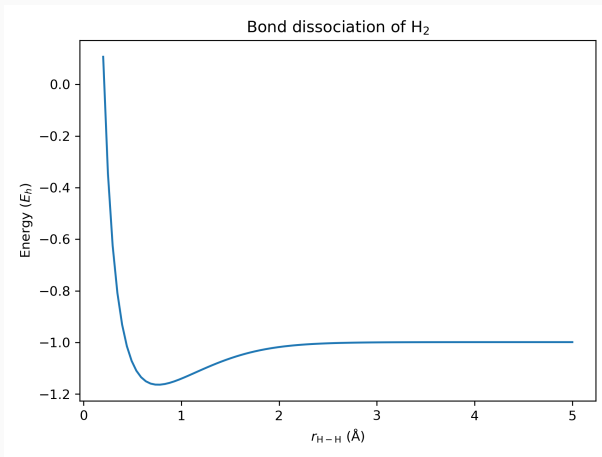
```
.PHONY: clean

clean:
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1  
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# An example use in scientific: $\text{H}_2$ dissociation

Let's write a real world example `Makefile`: the potential energy surface of the dissociation of  $\text{H}_2$  computed with `Psi4` at the CCSD/cc-pVDZ level.



## An example use in scientific: H<sub>2</sub> dissociation

To do this, we will:

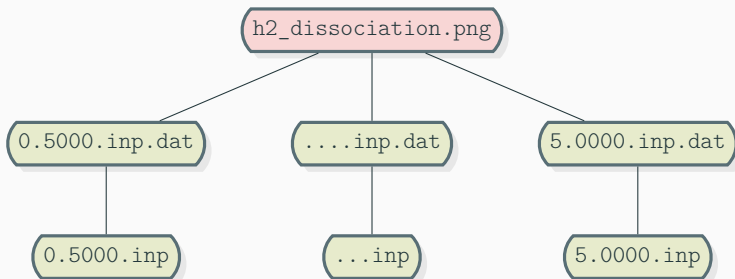
1. generate a set of input files from 0.2 Å to 5 Å
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# Conclusion

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1. `Make` is not so bad! It is just a bunch of dependency rules
2. It can help you drive computations efficiently, without rerunning stuff twice.
3. It is a tool that simplifies many different tasks, not only building software

## Related software

1. `snakemake`

<https://snakemake.readthedocs.io/en/stable/index.html>

2. `ninja` <https://ninja-build.org/>

3. `invoke` <http://www.pyinvoke.org/>