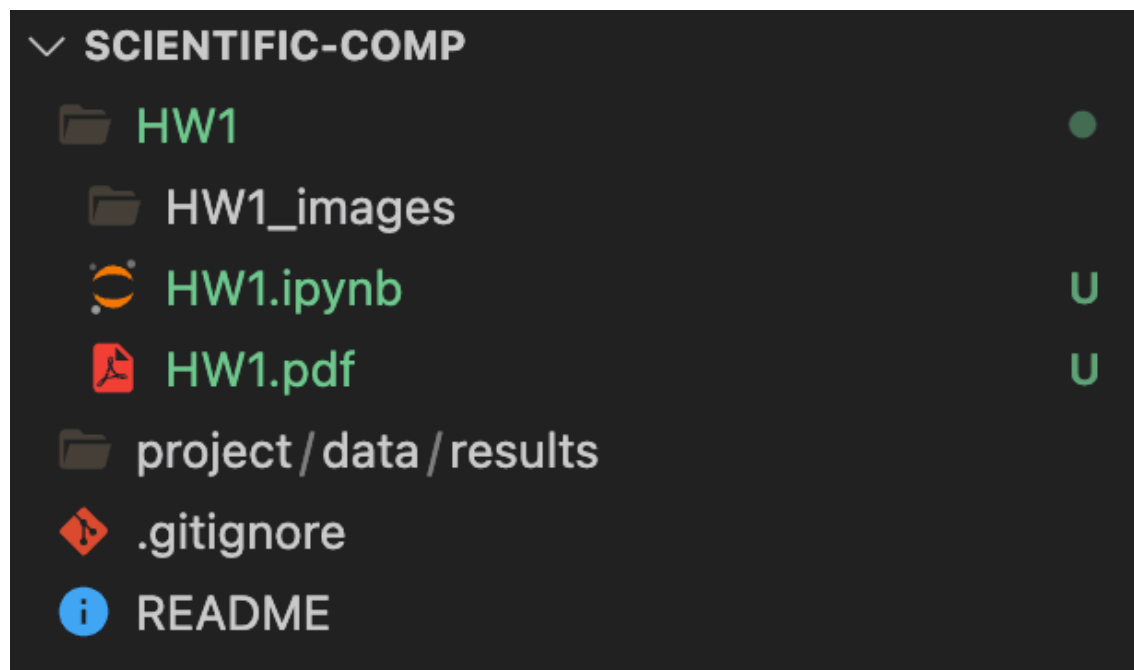


CMSC6950 Homework #1

Isaac Adoboe - ieadoboe@mun.ca

Before I start the assignment, I created this python notebook and a images folder to store the screenshots for the assignments. Below is how the folder looks now.

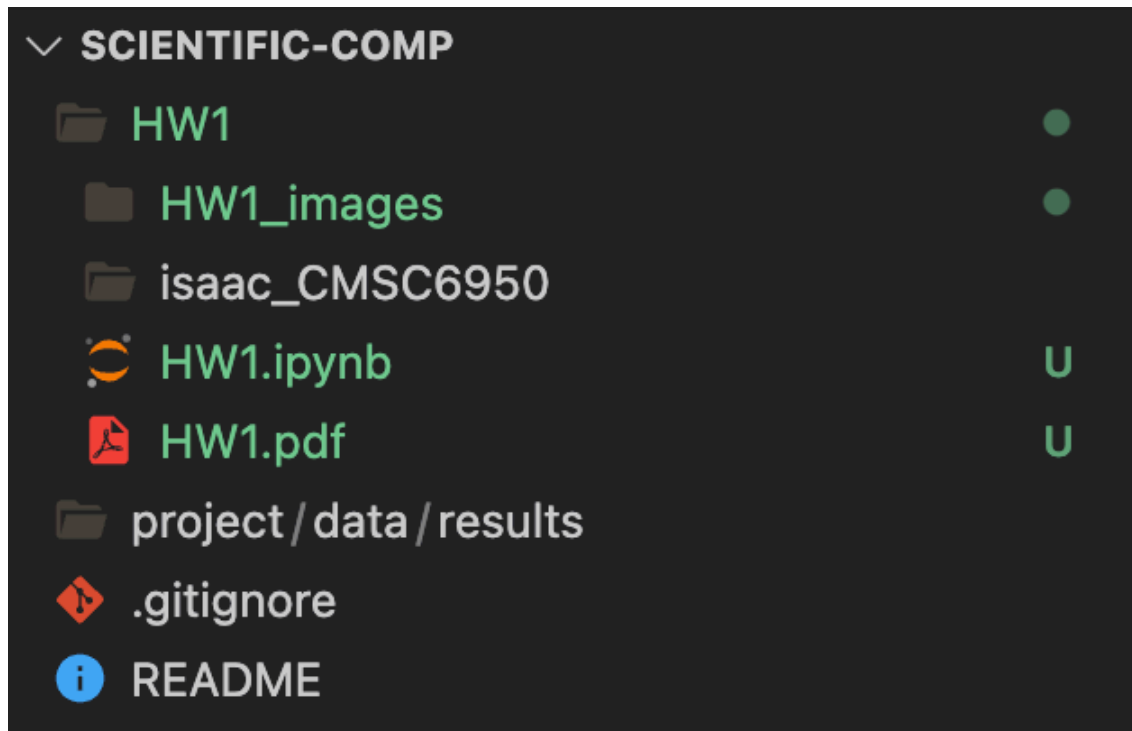
```
(base) isaacadoboe@mac ~ % cd Developer/scientific-comp/HW1
(base) isaacadoboe@mac HW1 % touch HW1.ipynb
(base) isaacadoboe@mac HW1 % mkdir HW1_images
```



Question 1

Make `isaac_CMSC6950` directory

```
(base) isaacadoboe@mac HW1 % mkdir isaac_CMSC6950
(base) isaacadoboe@mac HW1 % cd isaac_CMSC6950
(base) isaacadoboe@mac isaac_CMSC6950 %
```



Create `202384695` text file

```
(base) isaacadoboe@mac isaac_CMSC6950 % nano 202384695.txt
(base) isaacadoboe@mac isaac_CMSC6950 % ls -F
202384695.txt
(base) isaacadoboe@mac isaac_CMSC6950 % ls -l
total 8
-rw-r--r--@ 1 isaacadoboe  staff  10 Sep 19 22:30 202384695.txt
```

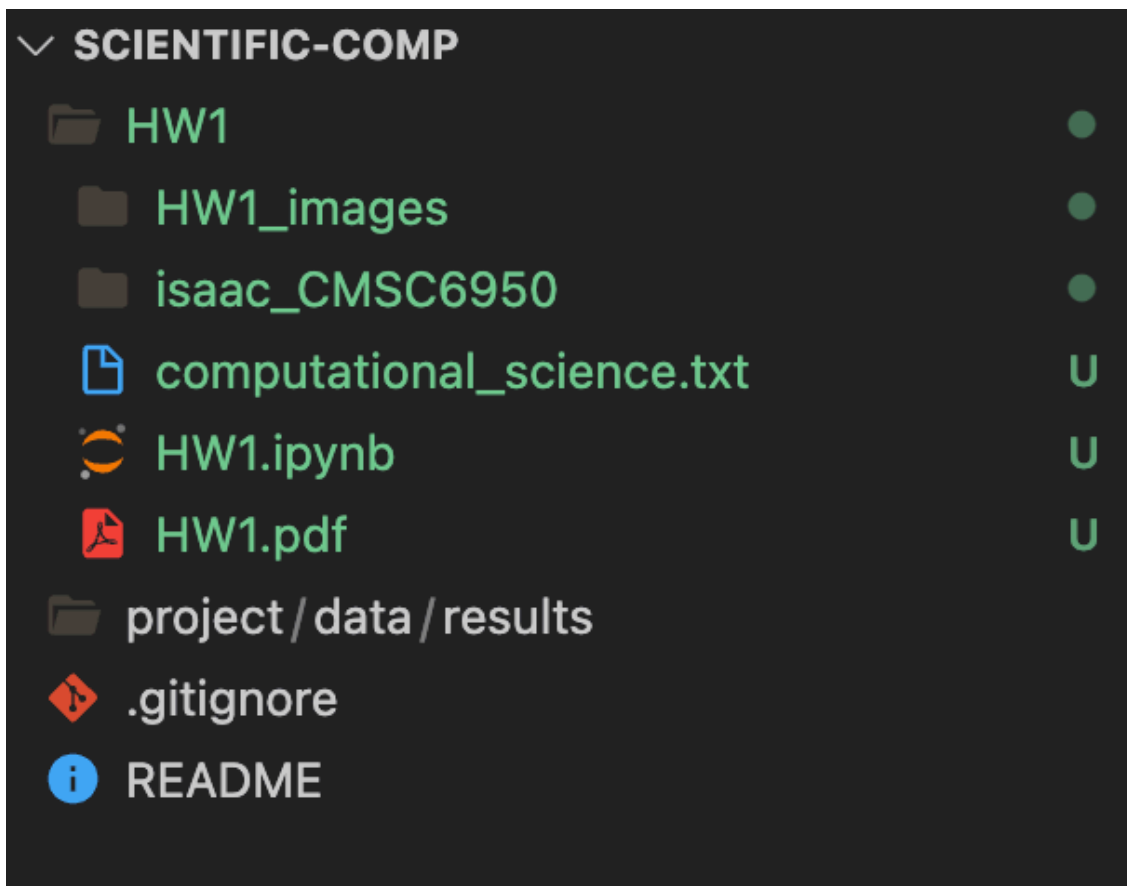
Show contents and change to home directory

```
(base) isaacadoboe@mac isaac_CMSC6950 % cat 202384695.txt
202384695
(base) isaacadoboe@mac isaac_CMSC6950 % cd ~
(base) isaacadoboe@mac ~ %
```

Question 2

Create `computational_science.txt` and renaming it

```
(base) isaacadoboe@mac HW1 % touch computational_science.txt
(base) isaacadoboe@mac HW1 % ls -l
total 1016
-rw-r--r--@ 1 isaacadoboe  staff      0 Sep 19 22:40 computational_science.txt
drwxr-xr-x@ 9 isaacadoboe  staff    288 Sep 19 22:35 HW1_images
-rw-r--r--@ 1 isaacadoboe  staff 448943 Sep 19 22:35 HW1.ipynb
-rw-r--r--@ 1 isaacadoboe  staff  68738 Sep 17 23:01 HW1.pdf
drwxr-xr-x@ 3 isaacadoboe  staff     96 Sep 19 22:30 isaac_CMSC6950
(base) isaacadoboe@mac HW1 % mv computational_science.txt computational_science.txt
(base) isaacadoboe@mac HW1 % ls -l
\total 1016
-rw-r--r--@ 1 isaacadoboe  staff      0 Sep 19 22:40 computational_science.txt
drwxr-xr-x@ 9 isaacadoboe  staff    288 Sep 19 22:35 HW1_images
-rw-r--r--@ 1 isaacadoboe  staff 448943 Sep 19 22:35 HW1.ipynb
-rw-r--r--@ 1 isaacadoboe  staff  68738 Sep 17 23:01 HW1.pdf
drwxr-xr-x@ 3 isaacadoboe  staff     96 Sep 19 22:30 isaac_CMSC6950
(base) isaacadoboe@mac HW1 %
```

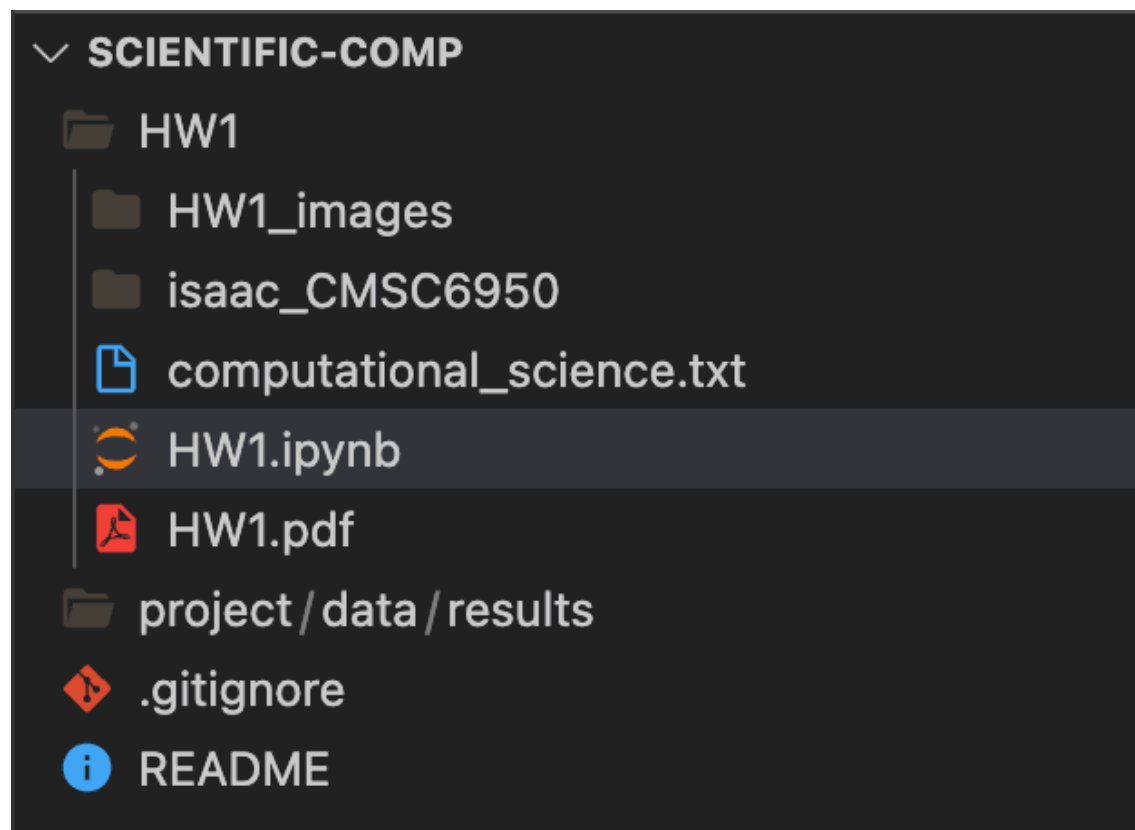


Remove `computational_science.txt` and create
`copmutational_science.txt`

```
(base) isaacadoboe@mac HW1 % rm computational_science.txt
(base) isaacadoboe@mac HW1 % touch computational_science.txt
(base) isaacadoboe@mac HW1 % ls -l
total 1640
-rw-r--r--@ 1 isaacadoboe  staff      0 Sep 19 22:48 computational_science.txt
drwxr-xr-x@ 11 isaacadoboe  staff    352 Sep 19 22:43 HW1_images
-rw-r--r--@ 1 isaacadoboe  staff  769092 Sep 19 22:47 HW1.ipynb
-rw-r--r--@ 1 isaacadoboe  staff   68738 Sep 17 23:01 HW1.pdf
drwxr-xr-x@ 3 isaacadoboe  staff     96 Sep 19 22:30 isaac_CMSC6950
(base) isaacadoboe@mac HW1 % cp computational_science.txt computational_science.txt
(base) isaacadoboe@mac HW1 % ls
computational_science.txt      HW1_images      HW1.pdf
computational_science.txt      HW1.ipynb       isaac_CMSC6950
(base) isaacadoboe@mac HW1 % rm computational_science.txt
(base) isaacadoboe@mac HW1 %
```

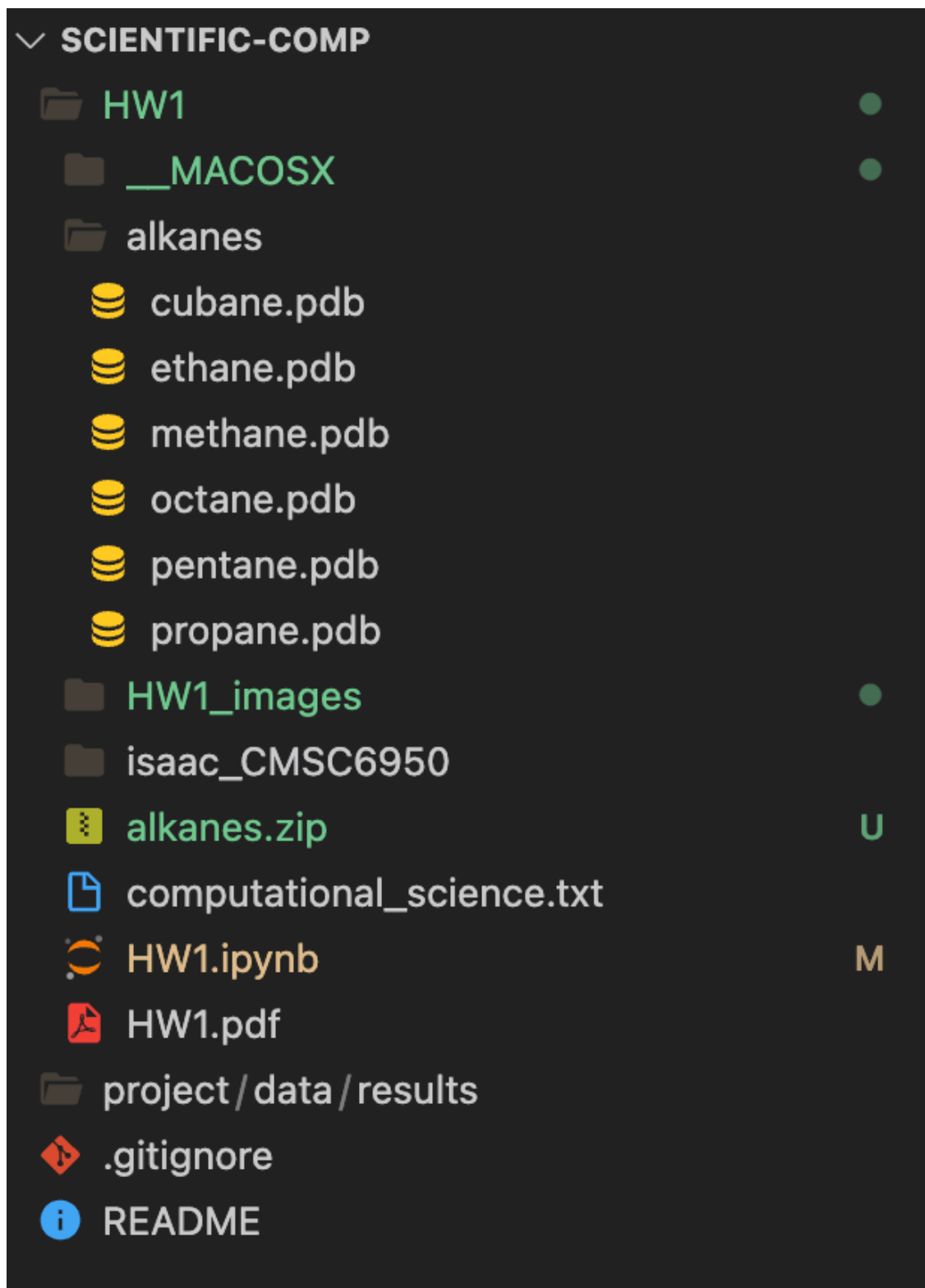
Question 3

Before adding the `alkanes` folder



Copy `alkanes.zip` folder to working directory and unzipping

```
(base) isaacadoboe@mac HW1 % cp ~/Downloads/alkanes.zip .
(base) isaacadoboe@mac HW1 % ls -l
total 2216
-rw-r--r--@ 1 isaacadoboe  staff    5306 Sep 19 22:59 alkanes.zip
-rw-r--r--@ 1 isaacadoboe  staff      0 Sep 19 22:49 computational_science.txt
drwxr-xr-x@ 13 isaacadoboe  staff    416 Sep 19 22:58 HW1_images
-rw-r--r--@ 1 isaacadoboe  staff 1054776 Sep 19 22:58 HW1.ipynb
-rw-r--r--@ 1 isaacadoboe  staff   68738 Sep 17 23:01 HW1.pdf
drwxr-xr-x@ 3 isaacadoboe  staff     96 Sep 19 22:30 isaac_CMSC6950
(base) isaacadoboe@mac HW1 % unzip alkanes.zip
Archive:  alkanes.zip
  creating: alkanes/
  inflating: __MACOSX/._alkanes/
  inflating: alkanes/propane.pdb
  inflating: __MACOSX/alkanes/._propane.pdb
  inflating: alkanes/octane.pdb
  inflating: __MACOSX/alkanes/._octane.pdb
  inflating: alkanes/cubane.pdb
  inflating: __MACOSX/alkanes/._cubane.pdb
  inflating: alkanes/ethane.pdb
  inflating: __MACOSX/alkanes/._ethane.pdb
  inflating: alkanes/pentane.pdb
  inflating: __MACOSX/alkanes/._pentane.pdb
  inflating: alkanes/methane.pdb
  inflating: __MACOSX/alkanes/._methane.pdb
(base) isaacadoboe@mac HW1 % cd alkanes
(base) isaacadoboe@mac alkanes %
```



Total number of lines in all files

```
isaacadoboe@mac ~/Developer/scientific-comp/HW1/alkanes
(base) > $ wc -l $(find . | grep pdb)
    15 ./propane.pdb
    30 ./octane.pdb
    20 ./cubane.pdb
    12 ./ethane.pdb
    21 ./pentane.pdb
     9 ./methane.pdb
   107 total
```

How many of the compounds have more than 6 atom's listed in their file?

```
isaacadoboe@mac ~/Developer/scientific-comp/HW1/alkanes
(base) > $ for file in *.pdb; do
    count=$(grep -c "ATOM" "$file")
    if [ $count -gt 6 ]; then
        echo "$file - $count"
    fi
done | wc -l
5
```

List the files in order of the decreasing number of lines.

```
isaacadoboe@mac ~/Developer/scientific-comp/HW1/alkanes
(base) > $ wc -l $(find . | grep pdb) | sort -nr
   107 total
    30 ./octane.pdb
    21 ./pentane.pdb
    20 ./cubane.pdb
    15 ./propane.pdb
    12 ./ethane.pdb
     9 ./methane.pdb
```

Question 4

(a) Begin with either the word "Meg" or the word "Jo"

```
isaacadoboe@mac ~/Developer/scientific-comp/HW1
(base) > $ grep -E "^(Meg|Jo)" LittleWomen.txt
Jo, who was a bookworm.
Jo immediately sat up, put her hands in her pockets, and began to
Jo was very tall, thin, and brown, and reminded one of a colt, for she
Jo gave a despairing groan, and Meg laughed outright, while Beth let
Jo, rolling her eyes and clutching at the air, as she had seen a famous
Jo was the first to wake in the gray dawn of Christmas morning. No
Meg with a "Merry Christmas," and bade her see what was under her
Meg was already covering the buckwheats, and piling the bread into one
Meg, as they set out their presents while their mother was upstairs
Jo in maroon, with a stiff, gentlemanly linen collar, and a white
Meg, who had a good many little 'aristocratic tastes' of her own.
Jo," returned the young lady.
Jo resigned herself with a sigh.
Jo quite glowed with pleasure at this boyish praise of her sister, and
Jo was her merry self again, because her dress was forgotten and nobody
Jo wanted very much to ask what his own way was, but his black brows
Jo thanked him and gladly went, wishing she had two neat gloves when
```

Jo led the way, and as if used to waiting on ladies, Laurie drew up a Jo told her adventures, and by the time she had finished they were at Jo laughed, Meg scolded, Beth implored, and Amy wailed because she Jo gave her sister an encouraging pat on the shoulder as they parted Jo happened to suit Aunt March, who was lame and needed an active Jo at a friend's, something in her comical face and blunt manners Jo's ambition was to do something very splendid. What it was, she had Meg was Amy's confidant and monitor, and by some strange attraction of Meg went back to toast her feet and read *Ivanhoe*, and Jo began to dig Jo liked his good breeding, and didn't mind having a laugh at Aunt Jo eagerly.

Jo, for her odd, blunt ways suited him, and she seemed to understand Jo, as she went up and down the walks, enjoying the blooming walls on Jo."

Meg could walk in the conservatory whenever she liked and revel in Jo opened the paper and began to laugh, for the first words she saw Jo let Laurie win the game to pay for that praise of her Beth, who Jo crossly, for she disliked the trouble of overseeing a fidgety child Meg and Beth said, "No." at once, and looked surprised. Amy poked the Meg flew to rescue Amy, and Beth to pacify Jo, but Jo was quite beside Jo wanted to lay her head down on that motherly bosom, and cry her Jo heard Amy panting after her run, stamping her feet and blowing on Jo's heart stand still with fear. She tried to call Laurie, but her Jo saw that her mother's eyes filled and her lips trembled as she Jo's only answer was to hold her mother close, and in the silence which Meg colored, but a mischievous fancy to tease the girls made her reply Meg couldn't refuse the offer so kindly made, for a desire to see if Meg smiled and relented, and whispered as they stood waiting to catch Meg danced and flirted, chattered and giggled, as the other girls did. Meg had told her adventures gayly and said over and over what a Meg."

Meg."

Jo went and sat on one arm of the chair, looking as if she thought they Meg's had roses and heliotrope, myrtle, and a little orange tree in it. Jo's bed was never alike two seasons, for she was always trying Jo's sudden change of tone made the girls laugh, but all looked rather Meg and Amy were contrary-minded, and Mr. Winkle rose to say with great Meg, coming home one warm day to find Jo laid upon the sofa in an Meg put out some of her sewing, and then found time hang so heavily, Meg ran upstairs and soon came back again, looking relieved but rather Jo, who knew still less than Meg about culinary affairs. Jo peeped into his half-open eye, felt his little heart, and finding Jo uttered a groan and fell back in her chair, remembering that she had Meg, in the other boat, was delightfully situated, face to face with Jo, and Ned. The English played well, but the Americans played better,

(b) Begin with the word "The" followed by a space

```
isaacadoboe@mac ~/Developer/scientific-comp/HW1
(base) > $ grep -E "^The\s" LittleWomen.txt
The Project Gutenberg EBook of Little Women, by Louisa May Alcott
The four young faces on which the firelight shone brightened at the
The clock struck six and, having swept up the hearth, Beth put a pair
The first sound in the morning was her voice as she went about the
The morning charities and ceremonies took so much time that the rest of
The boy sat down again and looked at his pumps, till Jo said, trying to
The old lady wouldn't speak to them for a time, but happening to meet
The moment Aunt March took her nap, or was busy with company, Jo
The idea amused Jo, who liked to do daring things and was always
The solitary, hungry look in his eyes went straight to Jo's warm heart.
The atmosphere of the whole house being summerlike, Laurie led the way
The old gentleman did not say much as he drank his four cups of tea,
```


The big house did prove a Palace Beautiful, though it took some time
The word 'limes' was like fire to powder, his yellow face flushed, and
The fifteen minutes seemed an hour, but they came to an end at last,
The storm cleared up below, for Mrs. March came home, and, having heard
The patience and the humility of the face she loved so well was a
The next day was fine, and Meg departed in style for a fortnight of
The Moffats were very fashionable, and simple Meg was rather daunted,
The garden had to be put in order, and each sister had a quarter of the
The P. O. was a capital little institution, and flourished
The unusual spectacle of her busy mother rocking comfortably and
The bread burned black; for the salad dressing so aggravated her that
The commander in chief and his aides soon spread the tablecloth with an
The Portuguese held his tongue like a brick, and walked the plank,
The story was not a long one, and when it was finished, he ventured to
The reader suddenly sat up, cast away the paper, displaying a flushed
The short afternoon wore away. All other errands were done, and Meg
The clocks were striking midnight and the rooms were very still as a
The rattle of an approaching carriage made them all start and listen.
The girls couldn't help laughing, and felt better for it, though Meg
The sight of the turnovers made Jo sober again; and when the two went
The girls are all as good as gold. Jo helps me with the sewing, and
The little girls are all well. Beth and my boy report daily. Hannah is
The good soul was wide awake in a minute, and took the lead at once,
The first of December was a wintry day indeed to them, for a bitter
The girls never forgot that night, for no sleep came to them as they
The little girl was very sincere in all this, for being left alone
The last name was written in pencil, and Amy explained that he was to
The kiss her mother gave her was a very tender one, and as she went
The shaggy eyebrows unbent a little as he rolled the steps toward the
The threat sounded awful, but did not alarm Jo, for she knew the
The note was written in the terms which one gentleman would use to
The invalids improved rapidly, and Mr. March began to talk of returning
The old lady couldn't resist her longing to see her nephew, for she had
The tea bell rang before he had finished describing the paradise which
The three years that have passed have brought but few changes to the
The girls gave their hearts into their mother's keeping, their souls
The last words were in answer to the look the elder lady gave him, a
The June roses over the porch were awake bright and early on that
The fatherly voice broke more than once, which only seemed to make the
The little house was not far away, and the only bridal journey Meg had
The invitations were sent, nearly all accepted, and the following
The lunch looked charming, and as she surveyed it, she sincerely hoped
The parlor windows were closed and curtained, no picture of the pretty
The little book was brought slowly out and laid down before him. Meg
The last words were spoken so low she thought he did not hear them, but
The family cardcase having done its duty the girls walked on, and Jo
The little girls hailed Amy and her treasures with delight, which
The art table was the most attractive in the room. There was a crowd
The fair was pronounced a success, and when May bade Amy goodnight, she
The Palais Royale is a heavenly place, so full of _bijouterie_ and
The sail up the Rhine was perfect, and I just sat and enjoyed it with
The baths at Nassau were very gay, so was Baden-Baden, where Fred lost
The pretty, modest girls are never talked about, except respectfully,
The color deepened in Jo's cheeks as she answered, with the look of
The plan was talked over in a family council and agreed upon, for Mrs.
The teaching would render her independent, and such leisure as she got
The maiden lady is a Miss Norton, rich, cultivated, and kind. She
The 'effalunt' sat up, looking as much in earnest as any of them, and
The girl had gone, and I thought he had also, it was so still, and I

(c) Contain a word with any letter, followed by qu followed by exactly six more

letters

```
isaacadoboe@mac ~/Developer/scientific-comp/HW1
(base) > $ grep -E "\b\wqu\w{6}\b" LittleWomen.txt
upon the little red squirmers as if they were unfledged angels.
Emmanuel or the Queen of the Sandwich Islands. The equipages are as
they found out that kicking and squalling brought them whatever they
squabbled about the cream."
feast. Squirrels were busy with their small harvesting. Birds
your equipment.
array of equipment including outdated equipment. Many small donations
```

(d) Ends with either the word "time" or "times" followed by a period.

```
isaacadoboe@mac ~/Developer/scientific-comp/HW1
(base) > $ grep -E "(time|times)\.$" LittleWomen.txt
rough hands with a sigh that any one could hear that time.
be, if we had no worries!" said Meg, who could remember better times.
"pecking" ended for that time.
time.
opinion of her, yet feeling ill at ease with him for the first time.
time.
you out every day, driving or walking, and we'll have capital times.
go out with him, when they walked and rode and had capital times.
times.
kindling for some time.
desire to laugh and cry at the same time.
don't like romps and flirts, though we may act as if we did sometimes.
Jo should go away for a time.
someone to tease, after his long abstinence from his favorite pastime.
be sure of her facts this time.
yourself, and let others go halves, as you always did in the old times.
```