

Linux&Vim Basic commands

Basic Linux Commands

A. File & Directory Navigation

| Command | Meaning | Examples |
|--|-------------------------------|---|
| <code>pwd</code> | Show current directory | <code>pwd</code> |
| <code>ls</code> / <code>ls -l</code> | List files / detailed listing | <code>ls</code> <code>ls -l</code> |
| <code>cd folder</code> | Change directory | <code>cd espresso/</code> <code>cd qe7.4/</code> |
| <code>cd ..</code> / <code>cd ~</code> | Go up / go to home | <code>cd ..</code> <code>cd ~</code> |

B. Create, Copy, Move, Delete Files/Folders

| Command | Meaning | Examples |
|---|----------------------|---|
| <code>mkdir folder</code> | Create new folder | <code>mkdir day1</code> <code>mkdir -p vm/linux_commands/</code> |
| <code>touch filename</code> | create a file | <code>touch test.in</code> <code>touch test2.in test3.in</code> |
| <code>rm filename</code> / <code>rm -r</code> | Delete file / folder | <code>rm test.in</code> <code>rm -r tmp_dir/</code> |
| <code>cp src dest</code> | Copy file or folder | <code>cp input.in input1.txt</code> <code>cp *.in day1/</code> |
| <code>mv src dest</code> | Move or rename | <code>mv input1.txt file.in</code> <code>mv file.in vm/</code> |

C. Viewing File Contents

| Command | Meaning | Examples |
|------------------------|---------------------------------|---|
| <code>cat file</code> | View entire file | <code>cat pw.out</code> <code>cat input.in</code> |
| <code>less file</code> | Scroll through file (q to quit) | <code>less pw.out</code> <code>/total energy</code> (search) |
| <code>head -n</code> | Show top N lines | <code>head -10 pw.out</code> <code>head -5 input.in</code> |
| <code>tail -n</code> | Show last N lines | <code>tail -20 pw.out</code> <code>tail input.in</code> |

D. Running Programs & Managing Processes

| Command | Meaning | Examples |
|---------------------------------------|-----------------------------------|---|
| <code>program < in > out</code> | Run a program with input/output | <code>pw.x < si.in > si.out</code> <code>dos.x < dos.in > dos.out</code> |
| <code>top</code> | See running processes | <code>top</code> (press <code>q</code> to quit) |
| <code>kill PID</code> | Stop a running process/force kill | <code>kill 1234</code> <code>kill -9 1234</code> |
| <code>chmod +x file</code> | Make file executable | <code>chmod +x run_qe.sh</code> |

E. Handy Tools

| Command | Meaning | Examples |
|---|-----------------------|--|
| <code>history</code> | Show past commands | <code>history</code> <code>!42</code> (re-run command 42) |
| <code>clear</code> | Clear terminal screen | <code>clear</code> <code>Ctrl + L</code> |
| <code>tar -zxvf filename</code> | untar tar file | <code>tar -zxvf day1.tar.gz</code> |
| <code>tar -zcvf name.tar.gz path</code> | create tar file | <code>tar -zcvf test.tar.gz .</code> |

VIM Quick Reference Sheet

A. VIM Modes – The Foundation

| Mode Name | How to Enter | What You Can Do | Tip or Example |
|---------------------|--|--|--|
| Normal Mode | Press <code>Esc</code> (default mode) | Navigate, delete, copy, run commands | Always press <code>Esc</code> to reset VIM |
| Insert Mode | Press <code>i</code> | Start typing text or code | Press <code>i</code> , type <code>Hello QE</code> , then <code>Esc</code> |
| Command Mode | Press <code>:</code> from Normal mode | Save, quit, search, run shell commands | <code>:wq</code> , <code>:q!</code> , <code>:set number</code> , <code>:!ls</code> |
| Visual Mode | Press <code>v</code> , <code>V</code> , or <code>Ctrl+v</code> | Select characters, lines, or blocks | Use for deleting or copying selected text |

B. Saving, Quitting, and Files

| Command | What It Does | Example or Tip |
|------------------|-----------------------------------|---|
| <code>:w</code> | Save the file | <code>:w</code> or <code>:w newfile.in</code> |
| <code>:q</code> | Quit (only if no unsaved changes) | <code>:q</code> |
| <code>:q!</code> | Force quit (discard changes) | <code>:q!</code> |
| <code>:wq</code> | Save and quit | <code>:wq</code> |

| Command | What It Does | Example or Tip |
|-----------------|--------------------------|-----------------|
| <code>:x</code> | Same as <code>:wq</code> | <code>:x</code> |

C. Navigation & Movement

| Command | What It Does | Example or Tip |
|----------------------|----------------------------------|--|
| <code>h j k l</code> | Move left, down, up, right | Use as arrow keys — <code>h</code> (←), <code>j</code> (↓), etc. |
| <code>G / gg</code> | Go to end/start of file | <code>G</code> = last line, <code>gg</code> = first line |
| <code>nG</code> | Go to line number <code>n</code> | <code>50G</code> jumps to line 50 |
| <code>/word</code> | Search forward | <code>/K_POINTS</code> , <code>/ecutwfc</code> , etc. |
| <code>n / N</code> | Repeat search forward/backward | <code>n</code> (next match), <code>N</code> (previous match) |

D. Editing, Deleting, Copying

| Command | What It Does | Example or Tip |
|---------------------------|-------------------------------|--|
| <code>x</code> | Delete character under cursor | Place cursor and press <code>x</code> |
| <code>dd</code> | Delete line | <code>3dd</code> deletes 3 lines |
| <code>yy</code> | Copy (yank) current line | <code>2yy</code> copies 2 lines |
| <code>p</code> | Paste after current line | <code>yy</code> → move → <code>p</code> |
| <code>u</code> | Undo last change | Press multiple times to undo more |
| <code>Ctrl + r</code> | Redo last undo | Use if you over-undo |
| <code>:s/old/new/g</code> | Replace all in file | <code>:s/scf/relax/g</code> , <code>:%s/O/H/g</code> |

E. Visual Mode – Select & Edit Like a Pro

| Mode/Key | What It Does | Example or Tip |
|----------------------------|--|--|
| <code>v</code> | Visual mode (select characters) | Move with <code>hjk l</code> , then press <code>y</code> to copy |
| <code>V</code> | Visual Line mode (select whole lines) | <code>V</code> , then <code>j</code> or <code>k</code> , then <code>d</code> to delete |
| <code>Ctrl + v</code> | Visual Block mode (columns) | <code>Ctrl + v</code> , select block, press <code>I</code> , type text, <code>Esc</code> |
| <code>d, y, p, ></code> | Apply delete/copy/paste/indent actions | Use after selecting with visual mode |
| <code>~</code> | Toggle case of selected text | Select and press <code>~</code> |

F. VIM Settings & Shell Access

| Command | What It Does | Example or Tip |
|---------|--------------|----------------|
|---------|--------------|----------------|

| Command | What It Does | Example or Tip |
|--------------------------|-----------------------------------|---|
| <code>:set number</code> | Show line numbers | Helps with debugging QE inputs |
| <code>:syntax on</code> | Enable syntax highlighting | Colours keywords and comments |
| <code>:!command</code> | Run shell command from within VIM | <code>!!ls</code> , <code>!pw.x < scf.in > scf.out</code> |

A quick vim test

Try creating a simple input file:

```
vim test.in      # open new file
i               # insert mode
(type a QE input block or random text)
Esc            # return to normal mode
:set number     # show line numbers
:wq            # save and quit
```