Computational Chemistry Using Linux

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Contents

1 Basic Commands

This document is a constantly changing and expanding guide to linux mainly for computational chemists but also for scientists in general, and perhaps for those interested in keeping up with the latest developments in the Fedora Linux distribution (current **version 28**).

Linux is an operating system which shares a very similar philosophy to that of **UNIX** [1]. There are many linux distributions (distros) and a place to check-out new ones and the status of the standard ones like Fedora, Ubuntu, SuSe, Slackware, Debian, etc, is distrowatch.com [2].

The first step in order to learn linux is to open a **terminal**.

Nowadays the terminal program is hidden more and more from the user, so this is the first effort that the new user has to make in linux. Once a terminal is running the user can start playing around with many commands. Perhaps the most valuable information that can be given to the new user at this point is on the existence of the command **man**. The **man** command shows you information on any linux/unix command, for example:

```
bash> man ls
```

Will show you information related to the list (**ls**) command. The **ls** command does just that, it lists the files in the folder you are positioned at. To know where you are located at, you can use the command **pwd** (print working directory), and to move away from there the command **cd** (change directory), for example:

```
bash> pwd
/home/username
bash> cd Desktop
bash> ls
Trash
```

2 Changes

Fedora 22 came with the great surprise that the *yum* package manager is being deprecated. The reasons for this are yet unknown to me, perhaps there is good reason as there was also good reason for systemd from Lennart Poettering, but, for now, just headache. The new package manager is called *dnf*.

- It seems to somewhat retain compatibility with yum.

- It's openSUSE code.

- It's supposed to be faster than yum but dnf updateinfo hangs forever.

The typical workflow of update, upgrade and install is retained:

2

```
bash> dnf update
bash> dnf upgrade
bash> dnf install emacs
```

3 Services

Starting with Fedora 15 a switch was made from the **sysvinit** system and service manager to **systemd**, so the services management administration has changed accordingly but for now one can still use **sysvinit**. One can find the scripts which start services at: */etc/init.d*.

You can call them directly like so:

```
sudo /etc/init.d/network stop
sudo /etc/init.d/network start
sudo /etc/init.d/network restart
```

3.1 sysvinit

Or you can call them using services:

```
sudo service network restart
```

You can also control which services get started or not at boot time depending on the runlevel that your system is going into with:

```
sudo chkconfig --levels 345 network on
```

You can also check the list of what services get turned on depending on runlevel with:

```
sudo chkconfig
```

3.2 systemd

The new way to control services in systemd is done using the command **systemctl**, so, for example to query the status and restart the httpd service you have to use the commands:

```
sudo systemctl status httpd.service
sudo systemctl restart httpd.service
```

To make a service start or not at boot-time you issue:

```
sudo systemctl enable mysqld.service
sudo systemctl disable mysqld.service
```

Fedora 24 by default does not start the **ssh** daemon, so you'll have to enable it for every time the system boots-up, and you'll also have to start **sshd**.

```
sudo systemctl enable sshd
sudo systemctl start sshd
```

And to list all services currently running in your system:

```
sudo systemctl status
sudo systemctl list-units
```

Fedora's description of the **systemd** system and service manager, **systemd** is at:
http://fedoraproject.org/wiki/Systemd

4 Network

4.1 NIS Client

In Fedora you have to :
include your nis server in /etc/sysconfig/network
    NISDOMAIN=nisserver.ki.se
    Then modify /etc/sysconfig/authconfig
    USENIS=yes
    To configure a NIS client you will have to modify the files:

    yp.conf nsswitch.conf
    According to how your administrator has setup your internal NIS.
    Sometimes your NIS may hang, supposedly you can change a little bit how things are organized in nss-witch.conf to make things move a little bit faster.

    https://bugzilla.redhat.com/show_bug.cgi?id=183188

    Detailed info at: http://www.server-world.info/en/note?os=Fedora_12&p=nis&f=2

4.2 NFS Server

Installing and configuring and NFS Server is somewhat simple if all ports are open as required and there are no issues installing NFS utilities. The following are the minimal steps needed in CentOS 7.

```
yum install nfs-utils libnfsidmap
systemctl enable rpcbind
systemctl enable nfs-server
systemctl start rpcbind
systemctl start nfs-server
systemctl start rpc-statd
systemctl start nfs-idmapd
exportfs -r
firewall-cmd --permanent --zone public --add-service mountd
firewall-cmd --permanent --zone public --add-service rpc-bind
firewall-cmd --permanent --zone public --add-service nfs
firewall-cmd --reload
```

```
emacs /etc/exports
      /home           10.1.0.0/255.255.0.0(async,rw,insecure,no_subtree_check)
```

4.3 NFS Client

```
sudo yum install autofs
sudo systemctl enable autofs.service
sudo chkconfig --level 345 autofs on
```

Make sure to look at /etc/auto.master to see if it's going to the export that has been setup at the NFS server side. You will also need to have a soft link calling the NFS exported partitions. e.g.

```
ln -s /net/myosin/u1 myosin/
```

    Verify boot time messages.

```
tail -100 /var/log/messages | grep automount
showmount -a
```

```
showmount -e beluga
showmount -e shamu
showmount -e 192.168.1.40
rpcinfo
```

One can have various problems with the NFS connection to audit them you can use:

```
df -F nfs
showmount -e shamu
showmount -e cod
nfsstat -c
rpcinfo -u shamu nfs
automount -t 3600
http://docstore.mik.ua/orelly/networking_2ndEd/nfs/ch09_02.htm
```

4.4 VPN Client

Configuring the VPN client in Fedora 14 is easy. Just go to System/Preferences/Network Connections. There you will find a VPN tab. In the VPN tab you choose to add a VPN connection and from the dropdown menu select Cisco compatible (vpnc). You will fill up the boxes with the following info:

```
Gateway: vpn.rutgers.edu
Group name: rutgers-ipsec
Group password: rutgers
User name: myusername
Domain: rci.rutgers.edu
```

And it's all done and you're "like" in Rutgers.

5   Packages

One important reason for linux distributions becoming more appealing to general (windows and mac) users since, say, ten years ago, is the genesis/development of package managers. The main package managers are *apt-get* (Debian-based or FreeBSD), and *yum* (RedHat based distributions - soon to be replaced by *dnf* but retains compatibility with yum).

The following is a list of frequently used yum functions:

```
yum list installed             #lists installed packages
yum erase xpdf                 #removes xpdf package
yum install xpdf               #installs xpdf package
yum search xpdf                #search in repo the keyword xpdf
```

It's good to update packages on a regular basis.

```
sudo yum update
```

Care should be taken on these automatic updates if there are special hardware configurations, say, a special graphics card, or a non-supported wireless device.

On installing a new Fedora I usually need the following packages.

```
sudo yum install emacs texlive texlive-texmf-fontsxdvi gv gvim gthumb
xpdf xfig  kile octave  R compat-gcc-34-g77.x86_64  emacs-ess avogadro
mysql-server  fontmatrix numpy  scipy  git meld  jython jmol  texmaker
scribes grace ffmpeg mencoder  bootchart geany sysstat mysql-workbench
phpMyAdmin netbeans rstudio tmux
```

For additional packages google "Mauriat Miranda Fedora".

```
sudo yum remove sendmail
sudo yum remove gnome-games
sudo yum remove evolution empathy
```

tmux: a terminal multiplexer
qtoctave: awesome gui for octave
hamster-applet: time tracking tool
meld: a diff like program for managing git merges when invoked by git mergetool
htop: An interactive version of top in colors.

5.1 Python

jython: Java like Python
pyopengl: OpenGL for python

```
sudo yum install scitools jython python-matplotlib PyOpenGL python-visual
```

5.2 Computational Chemistry

As a computational chemist you want to hit your molecular problem with as many tools as you can. In an ideal world perhaps all of the following programs would be available in a correctly set-up machine. Some of the following packages can be installed directly via yum (dnf), but many cannot. Some might even be windoze. Some are free, some are expensive.

```
FREE
==============================================================================

Viewers
------------------------------------------------------------------------------
avogadro:   a molecular viewer with openbabel integration
chimera:    molecular visualization from Thomas Ferrin
ifort:      intel fortran
jmol:       java like rasmol/pymol
king:       molecular visualization from Richardson's lab
molden:     for viewing quantum chemistry results
molekel:    for viewing quantum chemistry results
prekin:     generate files for king from pdb also from Richardson's
pymol:      can be installed with yum, but not latest version.
vmd:        molecular visualization from Schulten lab.


QC, MM, MD, PB-solvers, pKa
------------------------------------------------------------------------------
apbs:       for solving the poisson-boltzman
gamess:     quantum chemistry
gtkdynamo:  for running QC/MM from pymol
mopac:      semi-empirical quantum chemistry
pdb2pqr:    make pdb file into pqr format. q=charges, r=radius
pkatool:    interactive graphical compute pKa of proteins.


PAY
==============================================================================

Viewers
------------------------------------------------------------------------------
```

```
chemdraw:   best chemical cartoons
hyperchem:  molecular visualization some calculation -- windoze -- expensive
maestro:    from the schrodinger bundle 3D and 2D view and draw
poseview:   protein-ligand complexes in 2D



QC, MM, MD, PB-solvers, pKa, dockers
----------------------------------------------------------------------------
adf:        mainly DFT quantum chemistry
gaussian:   quantum chemistry
glide:      docker from schrodinger
jaguar:     q.m. from the schrodinger bundle
macromodel: md from the schrodinger bundle
desmond:    parallel md from the schrodinger bundle
turbomole:  DFT done right. It has the DFT-VdW of Maxime Dion and David Langreth.
```

6 Security

6.1 NO iptables for the future?. FirewallD a new XML based firewall

So, starting with fedora 18, they've decided to switch to another type of securing ports and services in Fedora. The new thing is called firewalld and, although quite ignorant about it for the time being, it smells like this is upper red-hat, NSA influenced.
Google "fedora firewalld" for info.
Reading more into this there seems to be a general opinion that the main difference between iptables and firewalld is on how the configuration of rules is taken care of. In firewalld XML configuration takes over.

To stop firewalld if needed use systemd:

```
systemctl status firewalld
systemctl stop firewalld
```

6.2 TCPWrappers

To completely close all your connections the first line of defense against intruders is TCPWrappers. You just have to make sure that the file /etc/hosts.deny has just one line, that is: ALL:ALL Which will stop all ip addresses from being able to connect to your computer. The next level of security is to open only those ports and protocols which you want to keep open to the outside world given a set of allowed ip addresses. You do this by modifying hosts.allow, for example:

```
ALL:127.0.0.1
sshd: .rutgers.edu
sshd: .ccb.rutgers.edu
sshd: 172.16.65.0/255.255.255.0
sshd: 172.16.23.0/255.255.255.0
```

6.3 iptables

To DROP all connections coming from a specific IP address.

```
iptables -A INPUT -s 43.229.53.12  -j DROP
service iptables save
```

Sometimes specific ports need to be opened, for example if one runs a Schrodinger license server one needs to open the ports 27008 and 53000. This can be done using the iptables command:

```
iptables -A INPUT -p tcp --dport 27008 -j ACCEPT
iptables -A INPUT -p tcp --dport 53000 -j ACCEPT
```

And then:

```
service iptables restart
```

or go to /etc/sysconfig and edit the iptables file adding the next two lines:
-A INPUT -s 192.168.0.0/16 -i eth1 -p tcp -m tcp –dport 27008 -m state –state NEW -j ACCEPT
-A INPUT -s 192.168.0.0/16 -i eth1 -p tcp -m tcp –dport 53000 -m state –state NEW -j ACCEPT
Notice that 192.168.0.0 means the range 192.168.* is open, the /16 means use all allowed addresses in 192.168.X.X, if one wanted just 192.168.0.X, then /24 at the end would be needed.
    After the change one must restart the firewall:

```
service iptables restart
```

6.4 ssh port

One way to drastically reduce the amount of attacks your server might be having is to change the address of the ssh port to a high number of your preference, for example, change it to port 3146. You just have to modify /etc/ssh/sshd_config.

6.5 SElinux

If you are using NFS as a client it's better to disable selinux. You will have to modify /etc/sysconfig/selinux to read disabled.
    But, to disable it also at the kernel level you will have to go to your grub configuration file, that is, /boot/-grub2/grub.cfg and append selinux=0 to it.
    Yet another nasty of selinux is its intrusiveness even at the filesystem level. Selinux does this by labeling the whole filesytem. The way to clean up the mess is with:

```
find / -print0 | xargs -r0 setfattr -x security.selinux 2>/dev/null
```

6.6 Close Unsecure Services

Perhaps the most unsecure service is the sendmail service, which you only use if you're a **mailserver**, not a mail client. You can go ahead and turn it off. In Fedora 16 and 17 another port 25 mail service is on by default, this one is called exim. You are not a mail-server and do not want to risk being a spam-bot, so also disable it.

```
#sudo chkconfig --level 2345 sendmail off
sudo systemctl disable sendmail
sudo systemctl disable exim
sudo service sendmail stop
sudo service exim stop
```

To check if it worked in fact, you will have to run nmap.

```
sudo yum install nmap
nmap localhost
```

7 Software Details

For some packages like R, of django, there are some additional packages on top of them that I have to install every time I get a new machine. I will just list them here.

7.1 MySQL

Two additional programs which make managing MySQL easier are MySQL workbench and phpMyAdmin. It is recommended to install both in your development machine.

After installing MySQL one has to create users and their corresponding passwords, but even before one has to check that mysql is running, and that it will be run at boot time.

```
sudo systemctl enable mysqld.service
sudo systemctl start mysqld.service
```

After that you have to login as root and create passwords.

```
mysql -u root
mysqladmin -u root password 'secret_password'
```

7.2 postgreSQL

Connecting to a database

```
$ psql postgres          # the default database
$ psql database_name
```

Connecting as a specific user

```
$ psql postgres john
$ psql -U john postgres
```

Connecting to a host/port (by default `psql` uses a unix socket)

```
$ psql -h localhost -p 5432 postgres
```

You can also explicitly specify if you want to enter a password `-W` or not `-w`

```
$ psql -w postgres
$ psql -W postgres
Password:
```

Once you're inside `psql` you can control the database. Here's a couple of handy commands

```
postgres=# \h               # help on SQL commands
postgres=# \?               # help on psql commands, such as \? and \h
postgres=# \l               # list databases
postgres=# \c database_name # connect to a database
postgres=# \d               # list of tables
postgres=# \d table_name    # schema of a given table
postgres=# \du              # list roles
postgres=# \e               # edit in $EDITOR
```

At this point you can just type SQL statements and they'll be executed on the database you're currently connected to.

7.2.1 User Management

Once your application goes into production, or basically anywhere outside of your dev machine, you're going to want to create some users and restrict access.

We have two options for creating users, either from the shell via `createuser` or via SQL `CREATE ROLE`

```
$ createuser john
postgres=# CREATE ROLE john;
```

One thing to note here is that by default users created with `CREATE ROLE` can't log in. To allow login you need to provide the `LOGIN` attribute

```
postgres=# CREATE ROLE john LOGIN;
postgres=# CREATE ROLE john WITH LOGIN; # the same as above
postgres=# CREATE USER john;            # alternative to CREATE ROLE which adds the LOGIN attribute
```

You can also add the `LOGIN` attribute with `ALTER ROLE`

```
postgres=# ALTER ROLE john LOGIN;
postgres=# ALTER ROLE john NOLOGIN;    # remove login
```

You can also specify multiple attributes when using `CREATE ROLE` or `ALTER ROLE`, but bare in mind that `ALTER ROLE` doesn't change the permissions the role already has which you don't specify.

```
postgres=# CREATE ROLE deploy SUPERUSER LOGIN;
CREATE ROLE
postgres=# ALTER ROLE deploy NOSUPERUSER CREATEDB;  # the LOGIN privilege is not touched here
ALTER ROLE
postgres=# \du deploy
           List of roles
 Role name | Attributes | Member of
-----------+------------+-----------
 deploy    | Create DB  | {}
```

There's an alternative to `CREATE ROLE john WITH LOGIN`, and that's `CREATE USER` which automatically creates the `LOGIN` permission. It is important to understand that users and roles are the same thing. In fact there's no such thing as a user in PostgreSQL, only a role with LOGIN permission

```
postgres=# CREATE USER john;
CREATE ROLE
postgres=# CREATE ROLE kate;
CREATE ROLE
postgres=# \du
                             List of roles
 Role name |                     Attributes                     | Member of
-----------+----------------------------------------------------+-----------
 darth     | Superuser, Create role, Create DB, Replication     | {}
 john      |                                                    | {}
 kate      | Cannot login                                       | {}
```

You can also create groups via `CREATE GROUP` (which is now aliased to `CREATE ROLE`), and then grant or revoke access to other roles.

```
postgres=# CREATE GROUP admin LOGIN;
CREATE ROLE
postgres=# GRANT admin TO john;
GRANT ROLE
postgres=# \du
                             List of roles
 Role name |                     Attributes                     | Member of
-----------+----------------------------------------------------+-----------
 admin     |                                                    | {}
 darth     | Superuser, Create role, Create DB, Replication     | {}
 john      |                                                    | {admin}
 kate      | Cannot login                                       | {}
postgres=# REVOKE admin FROM john;
REVOKE ROLE
postgres=# \du
```

```
                     List of roles
 Role name |                  Attributes                 | Member of
-----------+---------------------------------------------+-----------
 admin     |                                             | {}
 darth     | Superuser, Create role, Create DB, Replication | {}
 john      |                                             | {}
 kate      | Cannot login                                | {}
```

7.2.2 Querying a Table

To retrieve data from a table, the table is *queried*. An SQL SELECT statement is used to do this. The statement is divided into a select list (the part that lists the columns to be returned), a table list (the part that lists the tables from which to retrieve the data), and an optional qualification (the part that specifies any restrictions). For example, to retrieve all the rows of table weather, type:

```
SELECT * FROM weather;
```

Here * is a shorthand for "all columns". [1] So the same result would be had with:

```
SELECT city, temp_lo, temp_hi, prcp, date FROM weather;
```

The output should be:

```
     city      | temp_lo | temp_hi | prcp |    date
---------------+---------+---------+------+------------
 San Francisco |      46 |      50 | 0.25 | 1994-11-27
 San Francisco |      43 |      57 |    0 | 1994-11-29
 Hayward       |      37 |      54 |      | 1994-11-29
(3 rows)
```

You can write expressions, not just simple column references, in the select list. For example, you can do:

```
SELECT city, (temp_hi+temp_lo)/2 AS temp_avg, date FROM weather;
```

This should give:

```
     city      | temp_avg |    date
---------------+----------+------------
 San Francisco |       48 | 1994-11-27
 San Francisco |       50 | 1994-11-29
 Hayward       |       45 | 1994-11-29
(3 rows)
```

Notice how the AS clause is used to relabel the output column. (The AS clause is optional.)

A query can be "qualified" by adding a WHERE clause that specifies which rows are wanted. The WHERE clause contains a Boolean (truth value) expression, and only rows for which the Boolean expression is true are returned. The usual Boolean operators (AND, OR, and NOT) are allowed in the qualification. For example, the following retrieves the weather of San Francisco on rainy days:

```
SELECT * FROM weather
    WHERE city = 'San Francisco' AND prcp > 0.0;
```

Result:

```
     city      | temp_lo | temp_hi | prcp |    date
---------------+---------+---------+------+------------
 San Francisco |      46 |      50 | 0.25 | 1994-11-27
(1 row)
```

You can request that the results of a query be returned in sorted order:

```
SELECT * FROM weather
    ORDER BY city;

     city       | temp_lo | temp_hi | prcp |    date
---------------+---------+---------+------+------------
 Hayward       |      37 |      54 |      | 1994-11-29
 San Francisco |      43 |      57 |    0 | 1994-11-29
 San Francisco |      46 |      50 | 0.25 | 1994-11-27
```

In this example, the sort order isn't fully specified, and so you might get the San Francisco rows in either order. But you'd always get the results shown above if you do:

```
SELECT * FROM weather
    ORDER BY city, temp_lo;
```

You can request that duplicate rows be removed from the result of a query:

```
SELECT DISTINCT city
    FROM weather;

     city
---------------
 Hayward
 San Francisco
(2 rows)
```

Here again, the result row ordering might vary. You can ensure consistent results by using `DISTINCT` and `ORDER BY` together: [2]

```
SELECT DISTINCT city
    FROM weather
    ORDER BY city;
```

7.3 Django

As Django is becoming one of the favorite web-frameworks for web developers now it's easy to install using yum, and so are some of it's extensions. In my work I've needed pagination and table sorting, which now are standard in Fedora 16. To install just issue:

```
sudo yum install Django django-pagination django-sorting mod_wsgi
```

7.4 R packages

R packages can easily be installed either from their source, or if they are hosted in one of the cran repositories.

For programs which are not included in the repositories such as bio3d (an interface program to molecular dynamics results) one can do the following after downloading the source in tar.gz format:

```
R CMD INSTALL bio3d_*.tar.gz
```

Or for installing cran hosted packages:

```
R
>install.packages("clue")
```

Some useful programs for statistical analysis of structural results are:

```
clue                    #cluster ensembles
ggplot2                 #advanced graphics
clValid                 #cluster validation
Matrix                  #additional matrix utilities
plotrix                 #matrix plotting program
Cairo                   #grapic production libraries. e.g. pdf
```

7.5   Rapache

First have to make sure that apache is running and that will run on startup.

```
sudo chkconfig --level 345 httpd on
sudo systemctl enable httpd.service
sudo service httpd start
sudo systemctl start httpd.service
```

Also have to install the httpd development package to be able to install rapache.

```
sudo yum install httpd-devel
```

7.6   gitweb

To install git and gitweb in fedora is pretty simple:

```
sudo yum install git
sudo yum install gitweb
```

Now you have to modify the /etc/gitweb.conf and /etc/httpd/conf.d/git.conf. For gitweb.conf this is what I have:

```
$projectroot = '/var/www/html/';
$site_name = "RNA-BPSDB";
$my_uri = "/";
$home_link = '/';
@stylesheets = ("/git/static/gitweb.css");
$favicon = "/git/static/git-favicon.png";
$logo = "/git/static/git-logo.png";
```

And for git.conf:

```
#Alias /git /var/www/git
<Directory /var/www/html/git>
  Options +ExecCGI
  AddHandler cgi-script .cgi
  DirectoryIndex gitweb.cgi
</Directory>
```

Now you have to go to your site and make it into a git repository. You will also have to move the default gitweb.cgi to your folder.

```
cd /var/www/html
git init
git add .
git commit -a
cp -r /var/www/git/ /var/www/html/git/
```

Finally you have to modify your gitweb.cgi, which must be in the git folder you just copied in the previous step. You just have to find the our $projectroot variable, and modify it to the path of your git folder. In this perl script you can also modify the header and the footer for your gitweb repository.

7.7   Wordpress

Installing wordpress was amazingly easy. I just followed the steps at http://www.if-not-true-then-false.com/2010/install-wordpress-on-fedora-centos-red-hat-rhel and was done in a few minutes. Perhaps the only additional information relevant here is that I am using the virtual server configuration by creating .conf files in the /etc/httpd/conf.d folder.

7.8   Wine

Installing wine in Fedora 14 is a piece of cake, yum works right out of the box.

```
sudo yum install wine
```

Nonetheless the configuration is another story. And what might happen to your X11 after running wine, will, most likely, make you go into single user mode and back to X-mode to fix it. Worst case scenario you'll have to reboot. The interest of installing wine is that of being able to use acrobat professional to anotate pdf documents, that is, articles.

7.9   Apache Configuration

It is convenient to set up apache as a virtual web server, that way you can have various sites in one server. To do this you have to mimick the httpd.conf file (which is the main apache configuration file) with a mysite.conf file which resides in /etc/httpd/conf.d. You can have as many mysite.conf files as you like. Some security settings which are recommended are to deny folder indexing by changing your httpd.conf to:

```
<Directory "/yourvirtualsitesfolder/">
#    Options Indexes FollowSymLinks
    Options FollowSymLinks
    AllowOverride None
    Order allow,deny
    Allow from all
</Directory>
```

Where "Indexes" has been erased from options. There are various needs that will start adding up in your mysite.conf, for example telling it where the cgi-folder is at and to avoid giving freebies of info about your system by turning off server signature.

7.10   Latex

There are a good amount of latex editors for Linux today. Fortunately many of them can be installed automatically using yum in Fedora.
     To install them use:

```
sudo yum install texmaker
sudo yum install gummi
sudo yum install texmacs
sudo yum install kile
sudo yum install geany
```

I mainly use emacs to write my latex documents, but sometimes you can learn new tricks with these editors. In texmacs is nice to see that you can call various packages for your format, for example the Springer-Verlag format for books, nice!.

If you want to use the Nucleic Acids Research latex format for publishing you'll need to install additional packages:

```
sudo yum install texlive-wrapfig texlive-sttools texlive-multirow \
                 texlive-boxedminipage
```

It seems like as of fedora 17, texlive was stuck in the 2009 version. You will have to install from scratch the 2012 version which comes with a manager called tlmgr. For some packets, like slashbox, tlmgr can't help you at all. You'll have to download from the repositories and install to you path. In my case:

```
sudo cp -r slashbox /usr/share/texmf/tex/latex/
sudo cp -r slashbox /usr/local/texlive/2012/texmf-dist/tex/latex
sudo /usr/local/texlive/2012/bin/x86_64-linux/mktexlsr
```

An additional package used at the website www.writelatex.com is colorlistoftodos. It allows you to comment and highlight a document by using backslash todo.

some other comment but inline and not on the side

some comment using colorlistoftodos package

7.11   Gnome 3

To configure gnome 3 system setting you will need to run the configure tool as root, so you'll have to invoke it via command line.

```
sudo yum gnome-control-center
```

7.12   VNC

One of the default vnc-clients in fedora is tigervnc, but it's not very customizable. Another one is remmina, which is not installed by default.

```
sudo yum install remmina remmina-plugins*
```

8   Linux Tricks

Some general linux tricks here.

```
nohup command >& output.log &          #Send program to background
                                         be able to logout cleanly.
```

9   Fedora Tricks

When you install Fedora or any other distro you just have to deal with whatever type of "artwork" they give you for the splash screens on starting the gnome-desktop-manager (gdm). So, the trick to change this is to modify the xml file at:

```
emacs /usr/share/backgrounds/laughlin/default/laughlin.xml
```

To fit into the xml code the images you want.

10   Links

This is just a collection of googled links.

A description of problems and fixes from a user who's just gotten Fedora 15 into his/her laptop.
http://www.cs.bham.ac.uk/~axs/laptop/

11   Complaints

Going from Fedora 14 to Fedora 15 and 16 has been a road full, very full, of thorns. The first problem was on having Gnome 3 in Fedora 15 and also the switch to systemd, which makes you change all of what you're used to, I mean, it changes everything!, it's almost as a complete change in fundamentals, no more init levels, for example. Many things are broken in Fedora 15 and 16 by default, here is a list:

If you install qt3 the links will be broken. The necessary binaries are at /usr/lib64/qt-3.3/bin

```
Audio in Fedora 16, have  to modify modprobe manually to recognize HDA
Intel.
Video -pymol flickers-
Video -Gnome 3 worked on F15, not on F16-
Video -virtualbox kernel drivers broken in F16-
NFS -Have to manually fix autofs timeout-
```

You can start having issued with the gnome-keyring bs. To disable just go to .gnome2/keyrings and erase everything there. When you relaunch chrome, which will ask for the keyring, make sure to enter an empty password.

12   Missing in Linux

One of the things missing in Linux is an easy to use pdf editor, for example something which works like preview in Mac OSX, or like Adobe Acrobat. The task needed is very easy, or at least seamingly easy, that is, to be able to underline, highlight, and make margin notes on pdf articles which can be modified later on by just opening the pdf document. Such task can be acomplished easily with the mentioned softwares which are not available in Linux. So far I've triend the following in Linux but all fall short.

```
xournal    # makes unmodifiable permanent changes in pdf
okular     # same as xournal. Have to save in their format
ooffice    # bad rendering and translates it into its own format
gimp       # opens one page at a time
inkscape   # same as gimp
flpsed     # only good for writing text over
scribus    # imports pdf and shows only parts of the document
pdftk      # same story, does not natively change the pdf
pdfedit    # first have to export QTDIR=/usr/lib64/qt-3.3 to be able to
             compile it in Fedora 16. And it doesn't allow you to
             underline or annotate in a letter by letter fashion. It
             will select the full paragraph.
pdfstudio # need to pay to get rid of watermark, same as xournal.-
```

This paragraphs is just to test justification and line wrapping in gedit which I would like to work like in emacs

13   Administration Tools and Commands

There are a good amount of system monitoring tools in linux, perhaps the ones that are mostly used by me are top, and it's improved version, htop, but there are many others.

```
bash> vmstat 3                        # report virtual memory
bash> uptime                          # machine uptime
bash> pstree                          # tree of current processes
bash> iostat                          # cpu stats
bash> mpstat -P ALL                   # stats for multiple cpus
bash> iptraf-ng                       # network traffic monitor/ iptraf
```

http://www.cyberciti.biz/tips/top-linux-monitoring-tools.html

14   Virtual Machine Step-by-Step Installation Notes

Here are notes on installing Fedora 24 as a virtual machine using VirtualBox in Mac OS Yosemite. I've decided to download the XFCE spin, which is 1.13Gb in size and a live image. So once the space is given in the virtual machine for installation the live image runs directly, and quite smoothly. Then I just click on install to hard-drive

and follow the GUI. I create a root password and one user with administrative priviledges. After the installation to hard-drive is done I shutdown the live-image and change the settings in VirtualBox so that the iso image is not booted this time around. The final install size is 3.7 Gygabytes.

- First steps

  - ☑ Remove selinux and clean selinux tags
  - ☑ Add user to sudoers
  - ☑ dnf install emacs
  - ☑ update linux
  - ☑ add repos
  - ☑ Copy .bashrc and .inputrc files
  - ☑ erase useless folders
  - ☑ install guest additions

- Install scientific packages

  - ☑ dnf install pymol avogadro
  - ☑ rdkit
  - ☑ R, rstudio, latex

References

[1] Wikipedia Linux. http://en.wikipedia.org/wiki/Linux (2015).

[2] Distrowatch Linux distribution watch. http://distrowatch.com (2015).