ThreaDom

get domain parser
Manual at http://csbl.bmb.uga.edu/downloads/domainparser_manual/manual.html
Description at http://csbl.bmb.uga.edu/downloads/domainparser_manual/about.html
Download from http://csbl.bmb.uga.edu/downloads/download.php?file=closed_files/domainparser2.LINUX.gz
Upload to server
$ gunzip domainparser2.LINUX.gz

Install boost (protein, lotus and iris server)

```
wget http://sourceforge.net/projects/boost/files/boost/1.57.0/boost_1_57_0.tar.gz/download
tar zxvf
```

 # Test boost installation
Reference: http://www.boost.org/doc/libs/1_59_0/more/getting_started/unix-variants.html#build-a-simple-program-using-boost

```
c++ -I path/to/boost_1_59_0 example.cpp -o example
echo 1 2 3 | ./example
# Output is 3 6 9
```

May not be needed, but to install boost

```
alias python='/usr/bin/python2.7' (adding to .bash_profile)
./bootstrap.sh
./b2 &> b2.log & (takes about 20 minutes)
tail -f b2.log
```

Using boost

```
./configure --with-boost=/data/bap54/tools/boost_1_57_0
```

Install LAPACK (iris server - quite a beast)

```
wget http://www.netlib.org/lapack/lapack-3.5.0.tgz
tar zxvf lapack-3.5.0.tgz
cd lapack-3.5.0.tgz
mv make.inc.example make.inc

export PATH=$PATH:/data/bap54/tools/gcc-4.5/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/data/bap54/tools/gcc-4.5/lib64

make
```

"Could not find BLAS" error while testing!

Went inside its own BLAS folder and compiled it using 'make'
Threw another error related to COMPLEX16 after running for a while, however, following gives a reasonable output (with numbers in the second column)

```
python lapack_testing.py

cmake .
make (this actually builds all the .o files)
```

[Did not need to made changes as suggested at http://stackoverflow.com/questions/18828730/lapack-linking-error-recompile-with-fpic]
make blaslib || make clean
make || make all

Install xz

```
wget http://tukaani.org/xz/xz-5.2.0.tar.gz
tar zxvf xz-5.2.0.tar.gz
cd xz-5.2.0/
./configure --prefix=/rose/space1/tools_badri/tools/xz-5.2.0
make
make install
export LD_LIBRARY_PATH=/rose/space1/tools_badri/tools/xz-5.2.0/lib
```

Free Contact Installation (protein server - unsuccessful - try iris server)

Install XZ if needed

Install Boost (not just copy)

Try freecontact

```
./configure --with-boost=/data/bap54/tools/boost_1_57_0
```

Gfortran not found error

```
export PATH=$PATH:/data/bap54/tools/gcc-4.5/bin (adding to .bash_profile)
```

Not supplying this gives "Cannot compile a simple gfortran program" error!

```
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/data/bap54/tools/gcc-4.5/lib64 (adding to .bash_profile)
```

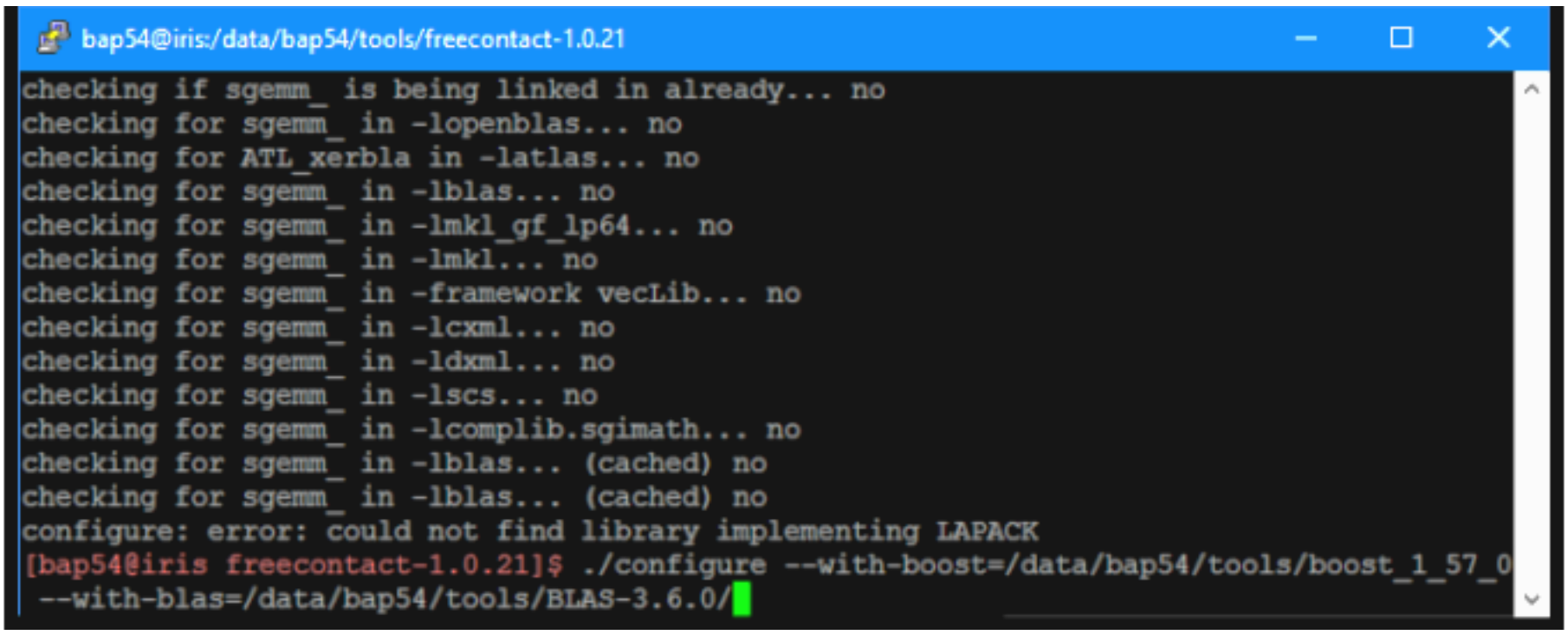
Supplying this gives early error “C++ compiler cannot create executables”

Supply the option but move the erroneous libraries to somewhere else
mv ../gcc-4.5/lib64/libstdc++.* ./temp/

Error “configure: error: could not find library implementing LAPACK”

./configure --with-boost=/rose/space1/bap54/temp/boost_1_57_0 --with-blas=/rose/space1/bap54/temp/lapack-3.5.0/librefblas.a
--with-lapack=/rose/space1/bap54/temp/lapack-3.5.0/liblapack.a

[configure: error: could not find library implementing LAPACK]



FreeContact (my local PC with Ubuntu 14.04)

```
$ wget ttp://http.debian.net/debian/pool/main/f/freecontact/freecontact_1.0.21.orig.tar.xz
$ sudo apt-get install libboost-all-dev
$ cd freecontact-1.0.21/
$ sudo ./configure --with-boost-libdir=/usr/lib/x86_64-linux-gnu
```

[found this reading here https://github.com/bitcoin/bitcoin/issues/3219]

install gfortran

```
$ apt-get update
$ apt-get install gfortran
```

install lapack

```
$ sudo apt-get update
$ sudo apt-get install libblas-dev checkinstall
$ sudo apt-get install libblas-doc checkinstall
$ sudo apt-get install liblapacke-dev checkinstall
$ sudo apt-get install liblapack-doc checkinstall

$ sudo ./configure --with-boost-libdir=/usr/lib/x86_64-linux-gnu
$ sudo make
$ sudo make all
$ sudo make install
$ export LD_LIBRARY_PATH=/usr/local/lib
```

[throws “error while loading shared libraries: libfreecontact.so.0:” otherwise]

test freecontact installation

```
$ freecontact < src/demo_1000.aln > contacts.txt
```

CCMPred (my local PC with Ubuntu 14.04)

Older version of this tool works.

```
$ sudo apt-get install cmake
$ wget https://github.com/soedinglab/CCMpred/archive/master.zip
$ unzip master.zip
$ cd CCMpred-master/
$ cmake .

# get libjanson
$ wget http://www.digip.org/jansson/releases/jansson-2.7.tar.gz
$ tar zxvf jansson-2.7.tar.gz
$ cd jansson-2.7/
$ sudo ./configure
$ sudo make
$ sudo make check
$ sudo make install

$ sudo apt-get install uuid-dev
$ make .
$ sudo apt-get update
$ sudo apt-get install msgpack
$ sudo apt-get install msgpack-python
$ sudo apt-get install libncurses-dev

$ cmake .
$ make
```

I find that the current downloadable of CCMpred has issues. Previous installation that I had downloaded earlier in lotus server went through the “cmake .” command. Currently getting - “Error running link command: No such file or directory”. Somehow it was fixed automatically.

Test ccmpred

```
$ ./bin/ccmpred example/1atzA.aln contacts.mat
```

PSI-BLAST (my local PC with Ubuntu 14.04)

MetaPSICOV needs PSIPRED which needs PSI-BLAST.

Reading instructions at ftp://ftp.ncbi.nih.gov/toolbox/ncbi_tools/README

```
$ wget ftp://ftp.ncbi.nih.gov/toolbox/ncbi_tools/ncbi.tar.gz
$ sudo apt-get install csh
$ sudo ncbi/make/makedis.csh
$ export PATH=$PATH:/home/badri/Downloads/ncbi/build
```

Reading the README at http://bioinfadmin.cs.ucl.ac.uk/downloads/psipred/FAQ I choose to install uniref90filt as the database.
Also there are a few notes here on formatting the DB https://www.biostars.org/p/70342/

```
$ wget ftp://ftp.ebi.ac.uk/pub/databases/uniprot/uniref/uniref90/uniref90.fasta.gz
```

$ gunzip -v uniref90.fasta.gz [makes the computer slow and eats up all the memory, looks like, around 5 minutes]
PSIPRED installation has the pfilt executable
$ bin/pfilt uniref90.fasta > uniref90filt [more than 10 minutes]

$ sudo apt-get install blast2 [for formatdb command]
$ which formatdb
/usr/bin/formatdb
$ formatdb -t uniref90filt -i uniref90filt [took abt 30 mins]
[not using blast+ so will do formatdb instead of makeblastdb]

$ which blastpgp
/home/badri/Downloads/ncbi/build/blastpgp
$ which makemat
/home/badri/Downloads/ncbi/build/makemat
$ which pfilt
/home/badri/Downloads/psipred/bin/pfilt

PSIPRED (my local PC with Ubuntu 14.04)

Followed instructions at http://bioinfadmin.cs.ucl.ac.uk/downloads/psipred/README
$ sudo apt-get install tcsh

Final configuration in the runspipred file:

```
# The name of the BLAST data bank
set dbname = /home/badri/Downloads/DB/uniref90filt

# Where the NCBI programs have been installed
set ncbidir = /home/badri/Downloads/ncbi/build

# Where the PSIPRED V2 programs have been installed
set execdir = /home/badri/Downloads/psipred/bin

# Where the PSIPRED V2 data files have been installed
set datadir = /home/badri/Downloads/psipred/data
```

$ cd example
../runpsipred example.fasta

HHSuite (my local PC with Ubuntu 14.04)

$ sudo apt-get install hhsuite
$ which hhblits
/usr/bin/hhblits
$ wget ftp://toolkit.genzentrum.lmu.de/pub/HH-suite/databases/hhsuite_dbs/uniprot20_latest.tar.gz
$ tar zxvf uniprot20_latest.tar.gz

PSICOV (my local PC with Ubuntu 14.04)

An issue is that we cannot download all files at once, although the main file we need is just psiccov21.c
$ mkdir psicov
$ cd psicov
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/CHANGELOG
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/LICENSE
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/Makefile
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/README
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/Version1/
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/demo.aln
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/demo.observed
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/demo.pdb
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/fasta2aln/
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/psicov21.c
$ wget -r http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/suppdata/

“make” did not work, so read this http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/README
$ gcc -O3 -march=native -ffast-math -m64 -ftree-vectorize -fopenmp psicov21.c -lm -o psicov
# Test the build
$ ./psicov demo.aln

MetaPSICOV (my local PC with Ubuntu 14.04)

Referred to the README at metapsicov/README

run_metapsicov × | runpsipredandsolv × | README × | .bashrc × | runpsipred ×

```
#!/bin/csh

# Change this to wherever you have installed the hhsuite library files
setenv HHLIB /home/badri/Downloads/hhsuite-2.0.9

# Edit to more sensible locations e.g. /usr/local
set metabindir = /home/badri/Downloads/metapsicov/bin
set metadatadir = /home/badri/Downloads/metapsicov/data

set sequence = $1
set target = $1:t:r

echo "Running PSIPRED+SOLVPRED..."

# Make sure you edit the runpsipredandsolv script with your local install information
runpsipredandsolv $1

# You will need to edit this line for your own hhblits installation directories etc.
# You may want to add extra parameters e.g. to enable multithreading.
hhblits -i $1 -d /home/badri/Downloads/DB/uniprot20_2013_03/uniprot20_2013_03 -oa3m $target.a3m -n 3 -
maxfilt 500000 -diff inf -id 99 -cov 60 > $target.hhblog
```

runpsipredandsolv × | run_metapsicov × | README × | .bashrc ×

```
#!/bin/tcsh

# This is a simple script which will carry out all of the basic
# required to make a PSIPRED V3 prediction plus a solvent acces
# prediction for MetaPSICOV. Note that it assumes that the
# following programs are in the appropriate directories:
# blastpgp - PSIBLAST executable (from NCBI toolkit)
# makemat - IMPALA utility (from NCBI toolkit)
# psipred - PSIPRED V3 program
# psipass2 - PSIPRED V3 program

# NOTE: This script is a replacement for the normal PSIPRED run
# assumes that PSIPRED has been already installed. Paths should
# to agree with your PSIPRED installation

# The name of the BLAST data bank you wish to use
set dbname = /home/badri/Downloads/DB/uniref90/uniref90filt

# Where the NCBI program binaries have been installed
set ncbidir = /home/badri/Downloads/ncbi/bin

#
# We assume here that the solvpred binary and weights_solv.dat
# installed in the same location as the PSIPRED binaries and da
# amended to whatever is the case on your installation.
#

# Where the PSIPRED V3 binaries have been installed
set execdir = /home/badri/Downloads/psipred/bin

# Where the MetaPSICOV binaries have been installed
set execdir2 = /home/badri/Downloads/metapsicov/bin

# Where the PSIPRED V3 data files have been installed
set datadir = /home/badri/Downloads/psipred/data

# Where the MetaPSICOV data files have been installed
set datadir2 = /home/badri/Downloads/metapsicov/data
```

Not a good experience of running metapsicov in my PC. When I run psiblast at the beginning, the computer already starts to slow down and freeze at times.

The new version of MetaPSICOV has some issues with the alnstats command. The error I get is

```
$ ./bin/alnstats
Segmentation fault (core dumped)
```

Copying an older version from lotus server, however, worked

```
$ ./bin/alnstats
*** Usage: alnstats alnfile singoutfile pairoutfile
```

```
$ date; ../run_metapsicov small.fasta; date
Sun Dec 20 14:26:32 CST 2015
Running PSIPRED+SOLVPRED...
Running PSI-BLAST with sequence small.fasta ...
Predicting secondary structure...
Pass1 ...
Pass2 ...
Solvation pass ...
Cleaning up ...
Final output files: small.ss2 small.horiz small.solv
```

Finished.
Running PSICOV...
Running freecontact...
Running CCMpred...
Output can be found in small.ccmpred
Running MetaPSICOV Stage 1...
Running MetaPSICOV Stage 2...
Running MetaPSICOV-HB...
Output files: small.metapsicov.stage1 small.metapsicov.stage2 small.metapsicov.hb
Sun Dec 20 14:43:32 CST 2015

PSICOV

Step1: Install psicov
---
wget -r -np -e robots=off http://bioinfadmin.cs.ucl.ac.uk/downloads/PSICOV/
cd bioinfadmin.cs.ucl.ac.uk/
find ./ -name index* -delete
cd downloads/PSICOV/
gcc -O3 -march=native -ffast-math -m64 -ftree-vectorize psicov21.c -lm -o psicov
./psicov

Step2: Install hhblits
---
wget ftp://toolkit.genzentrum.lmu.de/pub/HH-suite/hhsuite-latest-linux-x86_64.tar.gz
tar zxvf hhsuite-latest-linux-x86_64.tar.gz
cd hhsuite-2.0.16-linux-x86_64/
mkdir databases
cd databases/
#wget ftp://toolkit.genzentrum.lmu.de/pub/HH-suite/databases/hhsuite_dbs/uniprot20_2012_03.tar.gz

tar zxvf uniprot20_2012_03.tar.gz
cd ../temp/

Step3: Test (as suggested in the PSICOV README)

../tools_badri/hhsuite-2.0.16-linux-x86_64/bin/hhblits -i example.fasta -d ../tools_badri/hhsuite-2.0.16-linux-x86_64/databases/uniprot20_2012_03 -oa3m example.a3m -n 3 -diff inf -cov 60
egrep -v "^>" example.a3m | sed 's/[a-z]//g' | sort -u > example.aln
../tools_badri/PSICOV/psicov -p -d 0.03 example.aln > example.psicov

##
Error 1: "wget ftp://toolkit.genzentrum.lmu.de/pub/HH-suite/databases/hhsuite_dbs/uniprot20_2012_03.tar.gz" has some issues!

Search results will be written to 3tgi.hhr
Reading in 4200221 column state sequences with a total of 1239107776 residues
Iteration 1
Prefiltering database
.....
HMMs passed 1st prefilter (gapless profile-profile alignment) : 88876
HMMs passed 2nd prefilter (gapped profile-profile alignment)   :   3806
HMMs passed 2nd prefilter and not found in previous iterations :   3806
Scoring 3806 HMMs using HMM-HMM Viterbi alignment
..... 1000 HMMs searched
..... 2000 HMMs searched
..... 3000 HMMs searched

Error in hhblits: unrecognized HMM file format in 'BADVIZABA.hhm'.
Context:
' 111 O   GLY A 22   68.994 -61.748 -27.137 1.00 68.80   O
ATOM   112 N   PHE A 23   69.856 -62.366 -29.123 1.00 91.71   N
ATOM   113 CA PHE A 23   69.552 -61.073 -29.753 1.00 84.47   C '

PSIPRED

=> Step1: Install NCBI toolkit
Following the instructions at ftp://ftp.ncbi.nih.gov/toolbox/ncbi_tools/readme.unx
wget ftp://ftp.ncbi.nih.gov/toolbox/ncbi_tools/ncbi.tar.gz
tar zxvf ncbi.tar.gz
./ncbi/make/makedis.csh

=> Step2: Download and format uniref90 database
wget ftp://ftp.uniprot.org/pub/databases/uniprot/uniref/uniref90/uniref90.fasta.gz (takes around 3 hours)
gunzip uniref90.fasta.gz
/home/casp11/tools/psipred/src/pfilt uniref90.fasta > uniref90pfilt
/home/casp11/tools/blast-2.2.9/formatdb -t uniref90pfilt -i uniref90pfilt (if this is done, later blastpgp throws error!, still checking!)
/home/casp11/tools/hhmsacompro/tool/ncbi-blast-2.2.25+/bin/makeblastdb -dbtype prot -in uniref90pfilt -out uniref90pfilt (instead, I did this, referring to https://www.biostars.org/p/70342/)

=> Step3: Test blastpgp
/home/bap54/tools_badri/ncbi/bin/blastpgp -i /home/bap54/tools_badri/example.fasta -d ./using_makeblastdb/uniref90pfiltmakedb -o output.txt

=> Step4: Install psipred
wget http://bioinfadmin.cs.ucl.ac.uk/downloads/psipred/psipred3.5.tar.gz
tar zxvf psipred3.5.tar.gz
cd psipred/src
make
make install

=> Step5: Update the runpsipred file
```
cd /home/bap54/tools_badri/psipred
set dbname = /home/bap54/tools_badri/databases/uniref/using_makeblastdb/uniref90pfiltmakedb
# Where the NCBI programs have been installed
set ncbidir = /home/bap54/tools_badri/ncbi/bin
# Where the PSIPRED V2 programs have been installed
set execdir = /home/bap54/tools_badri/psipred/bin
# Where the PSIPRED V2 data files have been installed
set datadir = /home/bap54/tools_badri/psipred/data
```

=> Step6: Test psipred
cd example
../runpsipred ./example.fasta

CNS Suite

Obtain
Go to http://cns-online.org/cns_request/ and fill out the information.
Open your email and download http://cns-online.org/download/v1.3/cns_solve_1.3_all_intel-mac_linux.tar.gz because "wget" command from server does not work because of authentication failure!
Copy the file to server

Unzip and make changes
tar xzvf cns_solve_1.3_all_intel-mac_linux.tar.gz
mv .cns_solve_env_sh cns_solve_env.sh (Yeas, this file is hidden. It took me a while to figure this out!)
vim cns_solve_env.sh
 - change _CNSsolve_location_ to '/rose/space1/bap54/cns_dgsa4genome/programs/cns_solve_1.3'
vim cns_solve_env
 - change _CNSsolve_location_ to '/rose/space1/bap54/cns_dgsa4genome/programs/cns_solve_1.3' (yes, at both places)

Install
make install

To execute
source cns_solve_env.sh
./intel-x86_64bit-linux/bin/cns_solve < input.inp > output.out

To increase the value for ‘nrestraints’ (maximum number of restraints it can take), we need to change the code at line 60 of the module ‘cns_solve_1.3/modules/nmr/readdata’.
vim cns_solve_1.3/modules/nmr/readdata
- change 20000 to 200000 (by adding a zero)

CCMPred (lotus server)

Install cmake
wget http://www.cmake.org/files/v3.0/cmake-3.0.2-Linux-i386.tar.gz
tar zxvf cmake-3.0.2-Linux-i386.tar.gz
./cmake-3.0.2-Linux-i386/bin/cmake (check to see if it runs)

Install ccmpred
wget https://github.com/soedinglab/CCMpred/archive/master.zip
unzip master.zip
cd CCMpred-master/
../cmake-3.0.2-Linux-i386/bin/cmake .
make
./bin/ccmpred

Step3: Test ccmpred
---
cd example/
../bin/ccmpred **-t 4** 1atzA.aln output.mat
more output.mat

Notes:

(1) The alignment files (.aln) may be generated as that for psicov. The file formats are similar.
(2) I was able to copy the folder to iris server and simply run it directly!

'unzip' command in 'iris' server:

'iris' (possibly ArchLinux) does not have 'unzip' command. Following worked for me:

a. Downloaded p7zip from https://sourceforge.net/projects/p7zip/ and copied it to server
b. Untarred p7zip using `$ tar xjvf p7zip_15.09_x86_linux_bin.tar.bz2`
c. Unzipped master.zip using `$ ../p7zip/p7zip_15.09/bin/7za x master.zip -r`

Testing the CUDAMat library:

- Download the CUDAMat main package from https://github.com/cudamat/cudamat/archive/master.zip.
- Unzip the file 'master.zip' using the technique above.
- In the 'README.md' file there is a small piece of python example code. Create 'test.py' and paste contents in it.
- Python version is very important for executing the script 'test.py'. For the current CUDAMat installation in 'iris' server, python2.7 works.
- Test using `$ /usr/bin/python2.7 test.py`

Installing 'biopython' in 'iris' server:

- Download biopython from github
  - `wget https://github.com/biopython/biopython/archive/master.zip`
- Unzip using the p7zip tool
- Create an installation directory
- Enter the biopython directory and execute
  - `/usr/bin/python2.7 setup.py install --prefix=/home/bap54/biopython/install/`
- Test the installation
  - `/usr/bin/python2.7 setup.py test`
- Add the following to ~/.bash_profile
  - `export PYTHONPATH=$PYTHONPATH:/home/bap54/biopython/install/lib/python2.7/site-packages/`

Below are the errors encountered because of no access to device in cactus server. Renzhi, Jie and I worked on it to resolve the issue.

Iris server:

```
bap54@iris:~/temp
[bap54@iris temp]$ nvcc -V
nvcc: NVIDIA (R) Cuda compiler driver
Copyright (c) 2005-2011 NVIDIA Corporation
Built on Thu_Jan_12_14:41:45_PST_2012
Cuda compilation tools, release 4.1, V0.2.1221
```

Catus server:

```
bap54@localhost:~/temp
[bap54@localhost temp]$ nvcc -V
nvcc: NVIDIA (R) Cuda compiler driver
Copyright (c) 2005-2013 NVIDIA Corporation
Built on Wed_Jul_17_18:36:13_PDT_2013
Cuda compilation tools, release 5.5, V5.5.0
```

```
bap54@iris:/data/bap54
[bap54@iris bap54]$ nvidia-settings -q gpucoretemp
nvidia-settings: error while loading shared libraries: libgtk-x11-2.0.so.0: cannot open
e or directory
[bap54@iris bap54]$ nvidia-
nvidia-bug-report.sh  nvidia-settings       nvidia-smi            nvidia-xconfig
[bap54@iris bap54]$ nvidia-settings
nvidia-settings: error while loading shared libraries: libgtk-x11-2.0.so.0: cannot open
e or directory
[bap54@iris bap54]$ nvidia-smi
Fri Dec 11 10:06:59 2015
+------------------------------------------------------+
| NVIDIA-SMI 3.295.20   Driver Version: 295.20         |
|-------------------------------+----------------------+----------------------+
| Nb.  Name                     | Bus Id        Disp.  | Volatile ECC SB / DB |
| Fan   Temp   Power Usage /Cap | Memory Usage         | GPU Util. Compute M. |
|===============================+======================+======================|
| 0.  GeForce GTX 550 Ti        | 0000:05:00.0  N/A    |       N/A        N/A |
|  30%   53 C  N/A   N/A /  N/A |   0%    3MB / 1023MB | N/A      Default     |
|-------------------------------+----------------------+----------------------|
| 1.  GeForce GTX 550 Ti        | 0000:02:00.0  N/A    |       N/A        N/A |
|  30%   52 C  N/A   N/A /  N/A |   0%    3MB / 1023MB | N/A      Default     |
|-------------------------------+----------------------+----------------------|
| Compute processes:                                               GPU Memory |
|  GPU  PID     Process name                                       Usage      |
|=============================================================================|
|  0.           Not Supported                                                 |
|  1.           Not Supported                                                 |
+-----------------------------------------------------------------------------+
[bap54@iris bap54]$
```

```
bap54@localhost:~
\05:00.0 VGA compatible controller: NVIDIA Corporation GF100GL [Quadro 4000] (rev a1) (prog
06:00.0 VGA compatible controller: NVIDIA Corporation GF100GL [Quadro 4000] (rev a1) (prog-
[bap54@localhost ~]$ nvidia-smi
Fri Dec 11 10:38:47 2015
+------------------------------------------------------+
| NVIDIA-SMI 334.21     Driver Version: 334.21         |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|===============================+======================+======================|
|   0  Quadro 4000         Off  | 0000:05:00.0     Off |                  N/A |
| 40%   51C    P0    N/A /  N/A |      4MiB /  2047MiB |      0%      Default |
+-------------------------------+----------------------+----------------------+
|   1  Quadro 4000         Off  | 0000:06:00.0     Off |                  N/A |
| 40%   49C    P0    N/A /  N/A |      4MiB /  2047MiB |      0%      Default |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Compute processes:                                               GPU Memory |
|  GPU       PID  Process name                                     Usage      |
|=============================================================================|
|  No running compute processes found                                         |
+-----------------------------------------------------------------------------+
[bap54@localhost ~]$
```

export PYTHONPATH=/home/bap54/projects/project03/lib:/home/bap54/projects/project03/numpy-datasets:/home/bap54/projects/project03/cudamat-rbm/:/home/bap54/projects/project03/setuptools/lib/python2.7/site-packages

python2.7 setup.py install --prefix=/home/bap54/projects/project03/setuptools

Tested the nvcc compiler in iris and cactus server

$ nvcc test.cu
$ ./a.out

test.cu code from the book: CUDA by example

```
#include <stdio.h>
__global__ void kernel( void ){
}

int main( void ) {
    kernel<<<1,1>>>();
    printf( "Hello, World!\n" );
    return 0;
}
```

Issue when running param.cu in iris/cactus server

Strangely, the param.cu example in page 25 of the book (CUDA by Example) compiles in cactus server but not in iris server. However, even in cactus server it throws an error while running the object file. For running the code, download book.h from https://bitbucket.org/mrfright/cuda_by_example/get/bd759a6527ff.zip.

Error in cactus server:

```
[bap54@localhost temp]$ nvcc param.cu; ./a.out
unknown error in param.cu at line 11
[bap54@localhost temp]$
```

This was probably because I was running a newer code in older version of nvcc??

Error in iris server:

```
bap54@iris:~/temp
[bap54@iris temp]$ nvcc param.cu
/usr/bin/ld: /tmp/tmpxft_00001a8c_00000000-13_param.o: undefined reference to symbol 'pthread_
cancel@@GLIBC_2.2.5'
/usr/bin/ld: note: 'pthread_cancel@@GLIBC_2.2.5' is defined in DSO /lib/libpthread.so.0 so try
 adding it to the linker command line
/lib/libpthread.so.0: could not read symbols: Invalid operation
collect2: ld returned 1 exit status
[bap54@iris temp]$
```

This was probably because (a) I was running a newer code in older version of nvcc (b) In this server, libraries cannot be loaded??

The main problem between iris server and cactus server is the following. When trying to run the “test_cudamat.py” we get error in cactus server.

bap54@localhost:~/projects/project03

```
 1 import numpy as np
 2 import cudamat as cm
 3
 4 cm.cublas_init()
 5
 6 # create two random matrices and copy them to the GPU
 7 a = cm.CUDAMatrix(np.random.rand(32, 256))
 8 b = cm.CUDAMatrix(np.random.rand(256, 32))
 9
10 # perform calculations on the GPU
11 c = cm.dot(a, b)
12 d = c.sum(axis = 0)
13
14 # copy d back to the host (CPU) and print
15 print(d.asarray())
16
"test_cudamat.py" 16L, 334C
```

bap54@iris:~/temp

```
[bap54@iris temp]$ python2.7 test_cudamat.py
[[ 2043.22827148  2013.75683594  1995.25549316  2077.13623047
   1988.01831055  2039.42260742  2061.125       2059.01855469  2067.4753418
   2166.97949219  1993.27233887  2082.10717773  2086.33300781  2078.1784668
   1940.49804688  2028.40100098  2099.73779297  1991.02209473
   2161.29443359  2077.73413086  2090.84960938  2076.50830078
   2048.10229492  2002.56323242  1966.19421387  1993.82727051
   2058.80786133  1991.3614502   1959.7947998   2018.41772461
   2185.48022461  2058.45947266]]
[bap54@iris temp]$
```

bap54@localhost:~/projects/project03

```
[bap54@localhost project03]$ python2.7 test_cudamat.py
unknown error
Traceback (most recent call last):
  File "test_cudamat.py", line 4, in <module>
    cm.cublas_init()
  File "/opt/cudamat-rbm/cudamat.py", line 1069, in cublas_init
    CUDAMatrix.ones = CUDAMatrix(np.ones((MAX_ONES, 1), dtype=np.float32, order = 'F'))
  File "/opt/cudamat-rbm/cudamat.py", line 169, in __init__
    raise generate_exception(err_code)
cudamat.CUDAMatException: CUBLAS error.
[bap54@localhost project03]$
```

Test cudamat-rbm package installations using nose as instructed in the cudamat-rbm install notes at https://github.com/cudamat/cudamat/blob/master/INSTALL.md

```
$ wget https://pypi.python.org/packages/source/n/nose/nose-1.3.7.tar.gz#md5=4d3ad0ff07b61373d2cefc89c5d0b20b
$ tar zxvf nose-1.3.7.tar.gz
$ cd nose-1.3.7
$ python2.7 setup.py install --prefix=/home/bap54/temp/nose-1.3.7
$ export PYTHONPATH=$PYTHONPATH:/home/bap54/temp/nose-1.3.7/lib/python2.7/site-packages
$ ./bin/nosetests

$ mkdir test
$ cp /opt/cudamat-rbm/test_* test/
$ ./nose-1.3.7/bin/nosetests
```

Iris and cactus have different outputs:

```
bap54@localhost:~/temp
[bap54@localhost temp]$ ./nose-1.3.7/bin/nosetests
unknown error
Eunknown error
Eunknown error
E
======================================================================
ERROR: test suite for <module 'test_cudamat' from '/home/bap54/temp/test/test_cudamat.pyc'
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/home/bap54/temp/nose-1.3.7/lib/python2.7/site-packages/nose/suite.py", line 209,
un
    self.setUp()
  File "/home/bap54/temp/nose-1.3.7/lib/python2.7/site-packages/nose/suite.py", line 292,
etUp
    self.setupContext(ancestor)
  File "/home/bap54/temp/nose-1.3.7/lib/python2.7/site-packages/nose/suite.py", line 315,
etupContext
    try_run(context, names)
  File "/home/bap54/temp/nose-1.3.7/lib/python2.7/site-packages/nose/util.py", line 471, i
y_run
    return func()
  File "/home/bap54/temp/test/test_cudamat.py", line 7, in setup
    cm.cublas_init()
  File "/opt/cudamat-rbm/cudamat.py", line 1069, in cublas_init
    CUDAMatrix.ones = CUDAMatrix(np.ones((MAX_ONES, 1), dtype=np.float32, order = 'F'))
  File "/opt/cudamat-rbm/cudamat.py", line 169, in __init__
    raise generate_exception(err_code)
CUDAMatException: CUBLAS error.
-------------------- >> begin captured stdout << ---------------------
```

```
bap54@iris:~/temp
[bap54@iris temp]$ ./nose-1.3.7/bin/nosetests
.........................................../opt/cudamat-rbm/cuda_fgrads.py:47: RuntimeWarnin
g: divide by zero encountered in log
  f = -(np.multiply(targets,np.log(curr_probs)) + np.multiply((1-targets), np.log(one_minus_cu
rr_probs))).sum()
/opt/cudamat-rbm/cuda_fgrads.py:47: RuntimeWarning: invalid value encountered in multiply
  f = -(np.multiply(targets,np.log(curr_probs)) + np.multiply((1-targets), np.log(one_minus_cu
rr_probs))).sum()
.
----------------------------------------------------------------------
Ran 46 tests in 305.748s

OK
[bap54@iris temp]$
```

Adding a path to PYTHONPATH allows us to use import statement in python scripts.

Following the instructions at https://github.com/cudamat/cudamat/blob/master/INSTALL.md I tried to install cudamat myself locally to see if newer version of cudamat works. For that first we need to install setuptools at https://pypi.python.org/pypi/setuptools

```
$ wget https://bootstrap.pypa.io/ez_setup.py -O - | python2.7 - --user
$ python2.7 setup.py install --user
$ export PYTHONPATH=$PYTHONPATH:/home/bap54/.local/lib/python2.7/site-packages
$ wget https://github.com/cudamat/cudamat/archive/master.zip
$ 7za x master.zip -r
$ cd cudamat-master/
$ python2.7 setup.py install --user
$ export
PYTHONPATH=/home/bap54/.local/lib/python2.7/site-packages:/home/bap54/projects/project03/lib:/opt/numpy-datasets:/home/bap5
4/temp/nose-1.3.7/lib/python2.7/site-packages
$ cp build/lib.linux-x86_64-2.7/cudamat/* ./cudamat
$ ../temp/nose-1.3.7/bin/nosetests
```

Still getting similar error

```
bap54@localhost~/cudamat-master
[bap54@localhost cudamat-master]$ ../temp/nose-1.3.7/bin/nosetests
EE
======================================================================
ERROR: test suite for <module 'test_cudamat' from '/home/bap54/cudamat-master/test/test_cudamat.pyc'>
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/home/bap54/temp/nose-1.3.7/lib/python2.7/site-packages/nose/suite.py", line 209, in run
    self.setUp()
  File "/home/bap54/temp/nose-1.3.7/lib/python2.7/site-packages/nose/suite.py", line 292, in setUp
    self.setupContext(ancestor)
  File "/home/bap54/temp/nose-1.3.7/lib/python2.7/site-packages/nose/suite.py", line 315, in setupContext
    try_run(context, names)
  File "/home/bap54/temp/nose-1.3.7/lib/python2.7/site-packages/nose/util.py", line 471, in try_run
    return func()
  File "/home/bap54/cudamat-master/test/test_cudamat.py", line 6, in setup
    cm.cublas_init()
  File "/home/bap54/cudamat-master/cudamat/cudamat.py", line 1506, in cublas_init
    raise CUDAMatException('error initializing CUBLAS: (err=%u)' % err)
CUDAMatException: error initializing CUBLAS: (err=-2)
```

Also, the following basic test throws error again. This time it says something more, but basically it is the same error.

```
bap54@localhost:~/projects/project03
[bap54@localhost project03]$ python2.7 test_cudamat.py
Traceback (most recent call last):
  File "test_cudamat.py", line 4, in <module>
    cm.cublas_init()
  File "/home/bap54/.local/lib/python2.7/site-packages/cudamat-0.3-py2.7-linux-x86_64.egg/c
udamat/cudamat.py", line 1506, in cublas_init
    raise CUDAMatException('error initializing CUBLAS: (err=%u)' % err)
cudamat.cudamat.CUDAMatException: error initializing CUBLAS: (err=-2)
[bap54@localhost project03]$
```

There is a solution proposed at http://askubuntu.com/questions/538549/cudamat-testa-exception-error-initializing-cublas but it needs a root permission. Also I don't know exactly what this is doing.

`$ nvidia-smi -i 0 -q`
shows that both servers have 2 GPUs

Test if theano runs in iris server and cactus server!
The guide is at http://deeplearning.net/software/theano/install.html
It needs nose and setuptools, that we already have.

We need gfortran for installing scipy (gfortran and gcc libraries) which I copied from protein server.
`$ export PATH=$PATH:/home/bap54/projects/theano/gcc-4.6/bin`
`$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/home/bap54/projects/theano/lib64`

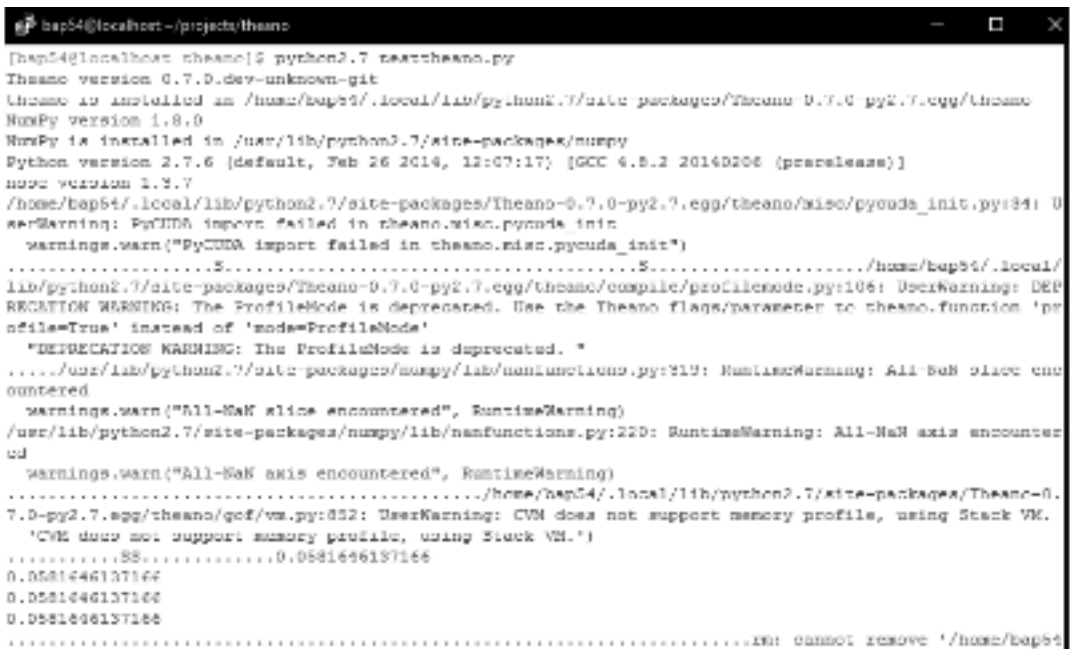
Install scipy:
```
$ wget http://sourceforge.net/projects/scipy/files/scipy/0.16.1/scipy-0.16.1.zip/download
$ mv download scipy.zip
$ 7za x scipy.zip -r
$ cd scipy-0.16.1
$ python2.7 setup.py install --user
```

Install theano:
```
$ wget https://github.com/Theano/Theano/archive/master.zip
$ mv master.zip theano.zip
$ 7za x theano.zip -r
$ python2.7 setup.py install --user
```

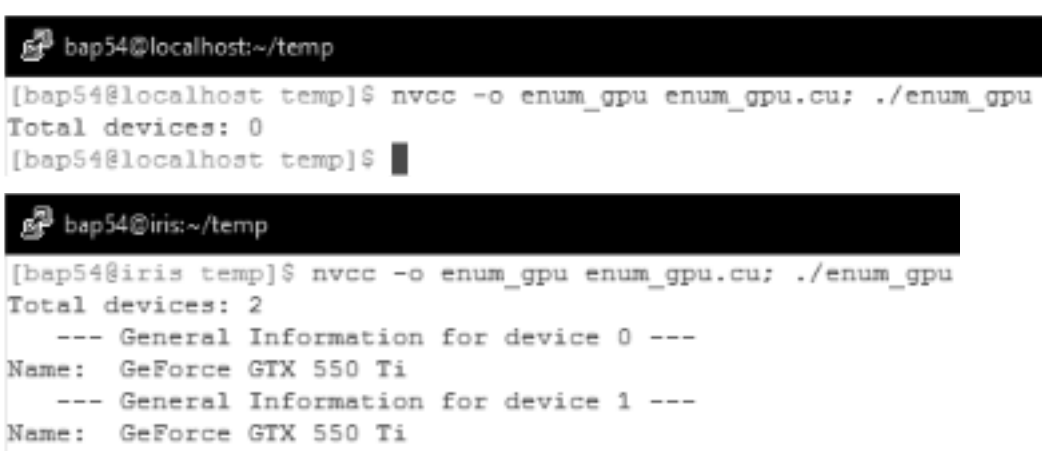
Test theano installation as suggested at http://deeplearning.net/software/theano/install.html#testing-your-installation
`$ vim testtheano.py`
```
import theano
theano.test()
```
Add nose path for testing
`$ export PYTHONPATH=$PYTHONPATH:/home/bap54/temp/nose-1.3.7/lib/python2.7/site-packages`

Theano can access GPU in iris server

```
bap54@iris:/data/bap54
[bap54@iris bap54]$ nvidia-smi
Tue Dec 15 16:09:25 2015
+------------------------------------------------------+
| NVIDIA-SMI 3.295.20   Driver Version: 295.20         |
|-------------------------------+----------------------+----------------------+
| Nb.  Name                     | Bus Id        Disp.  | Volatile ECC SB / DB |
| Fan   Temp   Power Usage /Cap | Memory Usage         | GPU Util. Compute M. |
|===============================+======================+======================|
| 0.  GeForce GTX 550 Ti        | 0000:05:00.0  N/A    |       N/A        N/A |
|  35%   65 C  N/A   N/A /  N/A |   6%   57MB / 1023MB |  N/A      Default    |
|-------------------------------+----------------------+----------------------|
| 1.  GeForce GTX 550 Ti        | 0000:02:00.0  N/A    |       N/A        N/A |
|  30%   46 C  N/A   N/A /  N/A |   0%    3MB / 1023MB |  N/A      Default    |
|-------------------------------+----------------------+----------------------|
| Compute processes:                                               GPU Memory |
|  GPU  PID     Process name                                       Usage      |
|==================================================================================|
|  0.           Not Supported                                                      |
|  1.           Not Supported                                                      |
+----------------------------------------------------------------------------------+
[bap54@iris bap54]$
```



Upon further investigation using the book's example I see that cuda does not find gpu devices in cactus server. Here is the output of the enum_gpu.cu code in cactus and iris server.



Installed CUDA in my local machine

At first installed the NVIDIA GeForce driver.

Mainly followed instructions at http://docs.nvidia.com/cuda/cuda-getting-started-guide-for-linux/#axzz3uEUJZhiB

Pre-installation actions
```
$ lspci | grep -i nvidia
$ uname -m && cat /etc/*release
$ gcc --version
```

Download the CUDA 7.5 toolkit from https://developer.nvidia.com/cuda-downloads
```
$ sudo dpkg -i cuda-repo-ubuntu1404-7-5-local_7.5-18_amd64.deb
$ sudo apt-get update
$ sudo apt-get install cuda
```

The last command threw error hence, did the following (reading at

http://askubuntu.com/questions/672047/anyone-has-successfully-installed-cuda-7-5-on-ubuntu-14-04-3-lts-x86-64)

```
$ sudo apt-get install libglew-dev libcheese7 libcheese-gtk23 libclutter-gst-2.0-0 libcogl15 libclutter-gtk-1.0-0
libclutter-1.0-0
```

Post-installation actions
```
$ export PATH=$PATH:/usr/local/cuda-7.5/bin
$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/cuda-7.5/lib64
```

Verify installation
```
$ cat /proc/driver/nvidia/version
$ nvcc -V
$ cd /usr/local/cuda-7.5/samples
$ make
```

Getting error:
```
badri@badri-ubuntu-Studio-XPS-8100:~/temp$ nvcc paran.cu
badri@badri-ubuntu-Studio-XPS-8100:~/temp$ ./a.out
CUDA driver version is insufficient for CUDA runtime version in paran.cu at line 11
badri@badri-ubuntu-Studio-XPS-8100:~/temp$
```

GPU and CUDA related configurations
```
$ lspci -v | grep -i nvidia
$ nvidia-settings -q NvidiaDriverVersion
$ uname -r
$ ./deviceQuery  (after doing the make on at CUDA folder's sample)
$ cat /proc/driver/nvidia/version
$ lsmod | grep -i nvidia
$ nvcc -V
$ nvidia-smi
```

Uninstalling
```
$ sudo apt-get remove --auto-remove nvidia-cuda-toolkit
```

After repeated install and uninstall of CUDA toolkit and nvidia driver, still could not fix the issue, so starting a fresh install of Ubuntu 14.04. By default, the open source Nouveau driver is installed. Gallium is a component of Nouveau.

Printing the manual http://docs.nvidia.com/cuda/pdf/CUDA_Getting_Started_Linux.pdf for reference.

Pre-installation actions:

wget http://developer.download.nvidia.com/compute/cuda/7.5/Prod/local_installers/cuda-repo-ubuntu1404-7-5-local_7.5-18_amd64.deb

```
$ sudo dpkg -i cuda-repo-ubuntu1404-7-5-local_7.5-18_amd64.deb
$ sudo apt-get update
$ sudo apt-get install cuda
```

The following packages have unmet dependencies:
cuda : Depends: cuda-7-5 (= 7.5-18) but it is not going to be installed
unity-control-center : Depends: libcheese-gtk23 (>= 3.4.0) but it is not going to be installed
Depends: libcheese7 (>= 3.0.1) but it is not going to be installed
E: Error, pkgProblemResolver::Resolve generated breaks, this may be caused by held packages.

Attempting Runfile Installation

```
# vim /etc/default/grub
```
# Uncomment to disable graphical terminal (grub-pc only)
GRUB_TERMINAL=console

sudo update-grub

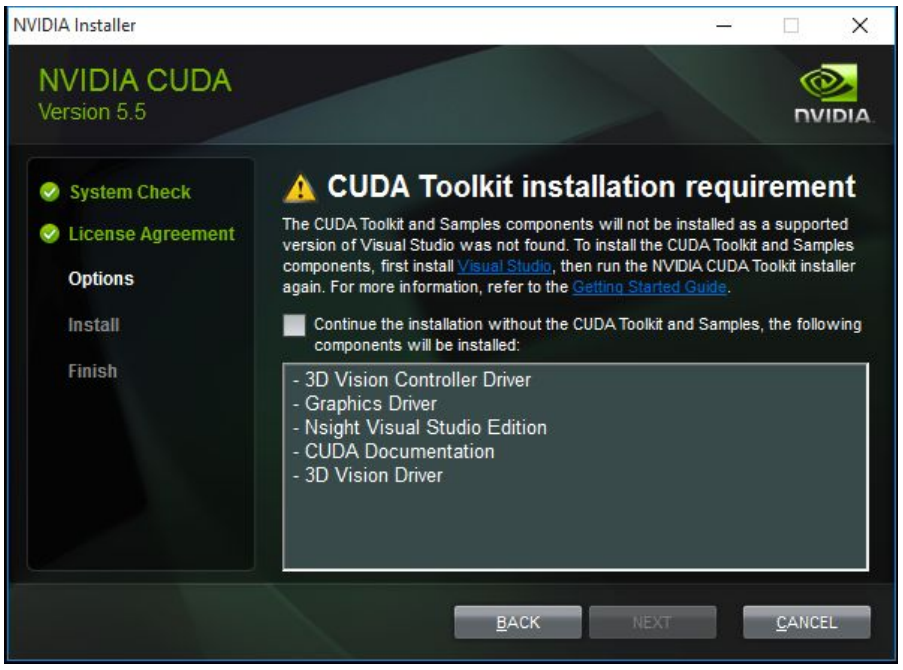
Removed ubuntu using the “bootrec /fixmbr” command as suggested at http://askubuntu.com/questions/133533/how-to-remove-ubuntu-and-put-windows-back-on. Worked successfully.

Trying CentOS installation now!

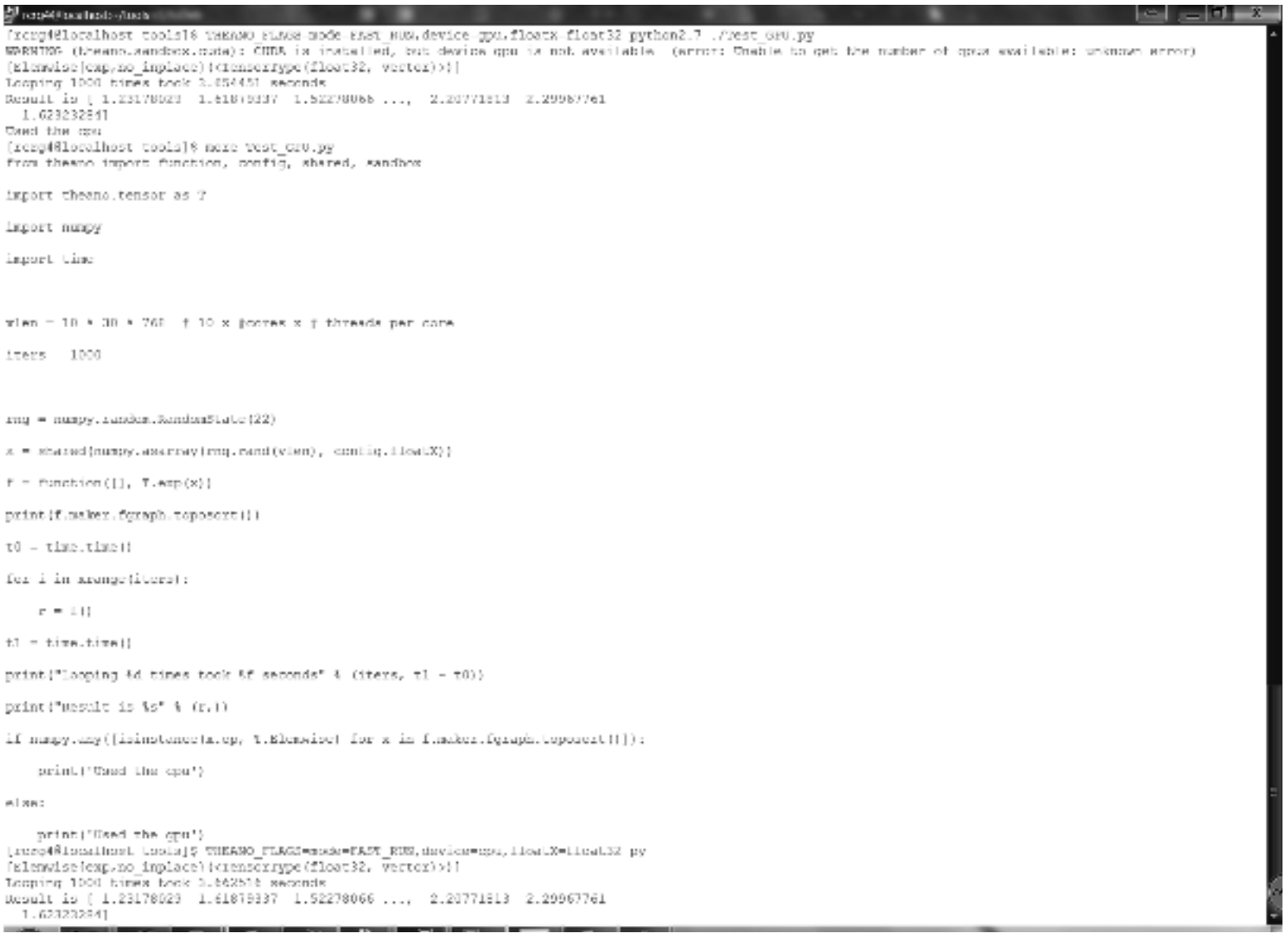
Satisfy dkms dependency
```
$ yum install epel-release
```

```
Follow the guide at http://docs.nvidia.com/cuda/pdf/CUDA_Getting_Started_Linux.pdf
$ sudo rpm --install cuda-repo….rpm
$ sudo yum clean expire-cache
```

In my local PC in windows, I got this error:



Jie Ho's and Renzhi's error message:



Rosetta Installation Notes (These notes were prepared in 2014 while installing Rosetta in lotus server):

1. Install scons

```
> wget http://prdownloads.sourceforge.net/scons/scons-2.3.0.tar.gz
> tar zxvf scons-2.3.0.tar.gz
> cd scons-2.3.0
> python setup.py install --prefix=/home/casp11/prototypes/prototype_of_rosetta3.5/scons-2.3.0
```

2. Download Rosetta3.5 (as one bundle of 1.6G) from https://www.rosettacommons.org/software/academic/

Username: Academic_User

Password: Xry3x4

(I downloaded the file to local machine and uploaded it to server. But you may copy it from within the server.)

```
> tar zxvf rosetta3.5_bundles.tgz
> cd /home/casp11/prototypes/prototype_of_rosetta3.5/rosetta-3.5/rosetta_source
# > ../../scons-2.3.0/bin/scons -D #bin
> scons bin mode=release
```

3. Try executing fragment picker

```
> /home/casp11/prototypes/prototype_of_rosetta3.5/rosetta-3.5/rosetta_source/bin/fragment_picker.linuxgccrelease
```

4. Setup sparks-x

a. Install blast

```
> wget ftp://ftp.ncbi.nih.gov/blast/executables/release/2.2.26/blast-2.2.26-x64-linux.tar.gz
> tar zxvf blast-2.2.26-x64-linux.tar.gz
```

b. Download nr database:

```
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.00.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.01.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.02.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.03.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.04.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.05.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.06.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.07.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.08.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.09.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.10.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.11.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.12.tar.gz
> wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.13.tar.gz
> for filename in *.tar.gz; do tar zxf $filename; done
```

c. Install Sparks-x (http://sparks.informatics.iupui.edu/yueyang/download/SPARKS-X/Readme)

```
> wget http://sparks.informatics.iupui.edu/yueyang/download/SPARKS-X/sparksx-1.tgz
> wget http://sparks.informatics.iupui.edu/yueyang/download/SPARKS-X/sparksx-1x.tgz
> wget http://sparks.informatics.iupui.edu/yueyang/download/SPARKS-X/sparksx-2.tgz
> wget http://sparks.informatics.iupui.edu/yueyang/download/SPARKS-X/sparksx-3.tbz
> tar -jxvf *.tbz
> tar zxvf sparksx-1.tgz
> tar zxvf sparksx-1x.tgz
> tar zxvf sparksx-2.tgz
> export SPARKSXDIR=/home/casp11/prototypes/prototype_of_rosetta3.5/sparks-x/sparks-x
> cd /home/casp11/prototypes/prototype_of_rosetta3.5/sparks-x/sparks-x
> ln -s /home/casp11/prototypes/prototype_of_rosetta3.5/psiblast/blast-2.2.26 ./blast
> ln -s /home/casp11/prototypes/prototype_of_rosetta3.5/DB/nr/ ./blast-NR
```

While making these soft links, old soft links may need to be renamed/removed

d. Test sparks-x

```
> ./bin/buildinp_query.sh ../../test/2lw7a.fasta
```

e. Sparks-x installation debug notes

i. In sysbio server, I got library missing error. I wa due to old Python version. I downloaded a newer version, installed it. I installed it with ./configure command parameterized to specific directory. And after installing added a line in ~/.bashrc file. The line looked like “export PATH=$newdir:$PATH”. Note that the new path is before all other paths.

ii. In sysbio server I got an error that said “invalid command cp –n”. I found that the file spineX.pl has a command cp with –n option. This –n needs to be changed to –f as a quick fix.

5. Install PsiPred (good documentation at http://www.biostars.org/p/70342/#70514)

a. Unzip psipred

```
> wget http://bioinfadmin.cs.ucl.ac.uk/downloads/psipred/old/psipred3.3.tar.gz
> tar zxvf psipred3.3.tar.gz
```

b. [Optional] Test psipred

i. Retrieve and format the uniref90 database

```
> wget ftp://ftp.uniprot.org/pub/databases/uniprot/uniref/uniref90/uniref90.fasta.gz
> gunzip -v uniref90.fasta.gz
> ./psipred3.3/bin/pfilt uniref90.fasta > unref90filt
```

Debug note: Instead of nr database, with this database name in $PFILTNR variable in make_fragments.pl “ObjMgrChoice” error is thrown, even though blast finishes. Don’t know why. It is most likely due to some disk/segment issues while running pfilt program. I remember reading something similar in a blog. But, this is not a problem now because the instructions for make_fragments.pl suggest to use nr database.

ii. ncbi toolkit (refer to the ./make/readme.unx for instructions)

```
> wget ftp://ftp.ncbi.nlm.nih.gov/toolbox/ncbi_tools/ncbi.tar.gz
> tar zxvf ncbi.tar.gz
> ./ncbi/make/makedis.csh
```

iii. Update directory paths for (1) dbname, and (2) ncbi toolkit in the runpsipred file

```
> vim ./psipred3.3/bin/runpsipred
```

Note: There should be no extra slash(“/”) at the end of the line beginning with ‘set ncbi’. It causes blastpgp to fail with segmentation fault error.

iv. Run runpsipred

```
> cd example
> ../runpsipred example.fasta
```

6. To Do: Install SAM, SAM-2nd and Porter

You will need to use at least two secondary structure predictions for fragment generation to make sense
https://www.rosettacommons.org/content/generate-structural-fragments
However, the comments in the file `make_fragment.pl` and the instructions in file `fragments.README` do not suggest that they are required. So, I am skipping them for now.

7. Setup make_fragments.pl

a. Download blast 2.2.17 (version matters for make_fragments.pl)

```
> wget ftp://ftp.ncbi.nih.gov/blast/executables/release/2.2.17/blast-2.2.17-x64-linux.tar.gz
> tar zxvf blast-2.2.17-x64-linux.tar.gz
```

b. Set Paths:

```
> export PERL5LIB=/home/casp11/prototypes/prototype_of_rosetta3.5/rosetta-3.5/rosetta_demos/public/homology_modeling_with_end_extension/scripts/cm_scripts/perl_lib
> export LD_LIBRARY_PATH=/home/casp11/prototypes/prototype_of_rosetta3.5/rosetta-3.5/rosetta_source/build/src/release/linux/2.6/64/x86/gcc/4.4/default/
```

c. Download PDB file list:

```
> wget ftp://ftp.wwpdb.org/pub/pdb/derived_data/pdb_seqres.txt
> wget ftp://ftp.wwpdb.org/pub/pdb/derived_data/index/entries.idx
```

d. Edit make fragments script (Guide is at https://www.rosettacommons.org/guide/Fragments)

Also a good documentation in the file `fragments.README`

```
> vim ./rosetta_tools/fragment_tools/make_fragments.pl
```

Update the following variables:

i. $BLAST_DIR
ii. $NR
iii. $PDB_SEQRES
iv. $PDB_ENTRIES_IDX
v. $FRAGMENT_PICKER
vi. $ROSETTA_DATABASE
vii. $SLAVE_LAUNCHER (To Do: Investigate how to run parallel!)
viii. $SPARKS
ix. $PSIPRED_DIR
x. $PSIPRED_USE_weights_dat4
xi. $PFILTNR

The original and updated .pl files are attached. Refer.

e. Test the updated make fragments script

```
> ./rosetta_tools/fragment_tools/make_fragments.pl -verbose 2akfa.fasta
```

8. Edit my scripts. Documentation for Abinitiorelax (recommended parameters) are discussed at
https://www.rosettacommons.org/manuals/archive/rosetta3.4_user_guide/d0/dd9/abinitio.html

a. a script that wraps fasta file according to Rosetta’s requirement, and

b. a script that makes use of make_fragments.pl and then runs Rosetta Abinitiorelax.

Find the scripts in the attached zip file.

9. Test by predicting structure for CASP5 target T0135. Compare the output with the native structure. The prediction should be close to the published paper displayed paper below.

```
> cd /rose/space1/common_tools/tools/rosetta3.5/
> mkdir test_T0135
> cd test_T0135/
> wget http://predictioncenter.org/casp5/targets/templates/t0135.seq.txt
> mv t0135.seq.txt t0135.fasta
> wget http://www.rcsb.org/pdb/files/1TR0.pdb
> /rose/space1/common_tools/tools/rosetta3.5/scripts/rosetta_predict.sh -f t0135 -n 10 -o /rose/space1/common_tools/tools/rosetta3.5/test_T0135
```

Test Results: