### UNIVERSITY OF TEXAS AT EL PASO COMPUTATIONAL SCIENCE (CPS)

#### A SHORT TUTORIAL

### Install Petsc-3.5.3 on My Desktop Show how to use PETSC on My Desktop and STAMPEDE

#### 1 References

http://www.mcs.anl.gov/petsc/index.html http://www.mcs.anl.gov/petsc/index.html -> Features

http://www.mcs.anl.gov/petsc/documentation/installation.html

http://acts.nersc.gov/petsc/

http://hpc.ucla.edu/hoffman2/software/petsc.php#cpp

http://charlesmartinreid.com/wiki/Petsc

http://parallel-programming-quickstart.blogspot.com/2007/10/installing-petsc.html

http://www.cise.ufl.edu/research/sparse/codes/

### 2 Introduction

PETSC stand for **P**ortable, **E**xtensible **T**oolkit for **S**cientific **C**omputation. it is pronounced PET-see, the S is silent. PETSC library is designed to work in both parallel and sequential codes, it is object orientated in design and is available for Linux (or Unix) and Windows. It consists of both data structures and functions that are intended for building scientific applications. **C**, **C**++, **Fortran** and **Python** are supported. In fact, PETSc includes a large suite of parallel linear, nonlinear equation solvers and ODE integrators that are easily used in application codes written in **C**, **C**++, **Fortran** and now **Python**. Also, PETSc is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. It supports MPI, shared memory pthreads, and GPUs through CUDA or OpenCL, as well as hybrid MPI-shared memory pthreads or MPI-GPU parallelism.

### 3 PETSC Important Features

PETSc has built in profiling for both memory usage and floating point calculation this accompanied with progress reporting features common in many of the solvers mean that one can get a reasonable picture of a codes execution profile merely by supplying a few additional command line arguments.

One of the strengths of the PETSc library is the large number of code examples it ships with. These examples are cross-referenced throughout the documentation so one can readily see an example of most significant functions along with related functions.

PETScs key feature is the number of highly regarded solvers etc. it brings under one roof: parallel timestepping ODE solvers, parallel preconditioners, Krylov subspace methods. parallel Newton-based nonlinear solvers and interfaces to numerous other 3rd party packages.

#### 4 Features include

- Parallel vectors
  - includes code for communicating ghost points
- Parallel matrices
  - several sparse storage formats
  - easy, efficient assembly

- Scalable parallel preconditioners
- Krylov subspace methods
- Parallel Newton-based nonlinear solvers
- Parallel timestepping (ODE) solvers
- Support for Nvidia GPU cards
- Complete documentation
- Automatic profiling of floating point and memory usage
- Consistent user interface
- Intensive error checking
- Portable to UNIX and Windows
- Over one hundred examples
- PETSc is supported and will be actively enhanced for many years

### 5 Find out if PETSC is installed already on your PC

You mat install already petsc on your PC using Synaptic Package Manager or sudo apt-get install petsc. If this is the case, you may want to know where is your PC petsc folder

```
>> echo petcs
petcs
>> whereis petsc
petsc: /usr/lib/petsc /usr/include/petsc
>> dpkg -l | grep petsc
ii libpetsc3.1
                                      3.1.dfsg-11ubuntu1
                                                                            Shared libraries for version 3.1 of PETSc
ii libpetsc3.1-dbg
                                     3.1.dfsg-11ubuntu1
                                                                            Static debugging libraries for PETSc \,
ii libpetsc3.1-dev
                                     3.1.dfsg-11ubuntu1
                                                                            Static libraries, shared links, header files for PETSc
ii petsc-dev
                                      3.1.dfsg-11ubuntu1
                                                                            Meta-package depending on latest PETSc development package
   petsc3.1-doc
ii
                                      3.1.dfsg-11ubuntu1
                                                                            Documentation and examples for PETSc
```

### 6 Install directly using apt-get or Synaptic Package Manager

There many ways to install PETSC. Here are two direct way, NO RECOMMENDED. Since PETSC requiere requiere to be configure to full fill your programming needs. These two way will not help to acomplish that.

• Open a terminal

```
>> sudo apt-get install petsc-dev
```

• Open Synaptic Package Manager, see figure (??)

### 7 Get PETSC on the follow wedsite

Open a terminal and create a folder where do you want to download PETSC. For example

```
>> cd Desktop/
>> mkdir PETSC
>> cd PETSC
```

Donwload petsc into the folder PETSC

henry@bluebottle:~/Desktop/PETSC\$ wget http://ftp.mcs.anl.gov/pub/petsc/release-snapshots/petsc-3.5.3.tar.gz

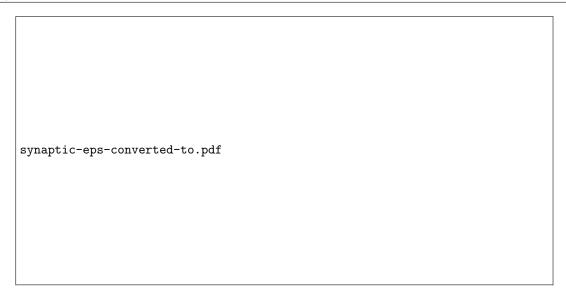


Figure 1: Synaptic Package Manager

```
Unpack PETSC in one step
henry@bluebottle:~/Desktop/PETSC$ gunzip -c petsc-3.5.3.tar.gz | tar -xof -
or
henry@bluebottle:~/Desktop/PETSC$ tar zxvf petsc-3.5.3.tar.gz
Unpack into two steps
henry@bluebottle:~/Desktop/PETSC$ gunzip petsc-3.5.3.tar.gz
henry@bluebottle:~/Desktop/PETSC$ tar xvf petsc-3.5.3.tar
henry@bluebottle:~/Desktop/PETSC$ cd petsc-3.5.3
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$
```

#### Get Examples for PETSC 8

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You use these examples to check if your PETSC installation and learn how to programming PETSC >> wget http://www.mcs.anl.gov/petsc/petsc-3.4/src/ksp/ksp/examples/tutorials/

# PETSC\_DIR and PETSC\_ARCH

Before run PETSc based program you must set two environment variables.

• Set PETSC\_DIR, first environment variable to the path of the PETSc directory. Within this directory there is a lib directory which will have at least one subdirectory corresponding to a set of PETSc libraries built with a given configuration.

```
export PETSC_DIR=~/Desktop/PETSC/petsc-3.5.3
```

Set PETSC\_ARCH, second environment variable is used to specify which library build within the PETSC\_DIR to use. This allows you to prepare a variety of PETSc builds e.g. optimised, debug differing MPI libraries etc. and create and run the corresponding executables while only changing the PETSC\_ARCH variable.

```
export PETSC_ARCH=linux-gnu-complex
```

• PETSC\_DIR and PETSC\_ARCH are a couple of variables that control the configuration and build process of PETSc. These variables can be set as environment variables or specified on the command line [to both configure and make].

- PETSC\_DIR: this variable should point to the location of the PETSc installation that is used. Multiple PETSc versions can coexist on the same file-system. By changing PETSC\_DIR value, one can switch between these installed versions of PETSc.
- PETSC\_ARCH: this variable gives a name to a configuration/build. Configure uses this value to stores the generated config makefiles in \${PETSC\_DIR}/\${PETSC\_ARCH}/conf. And make uses this value to determine this location of these makefiles [which intern help in locating the correct include and library files].
- Thus one can install multiple variants of PETSc libraries by providing different PETSC\_ARCH values to each
  configure build. Then one can switch between using these variants of libraries [from make] by switching the
  PETSC\_ARCH value used.
- If configure doesn't find a PETSC\_ARCH value [either in env variable or command line option], it automatically generates a default value and uses it. Also if make doesn't find a PETSC\_ARCH env variable it defaults to the value used by last successful invocation of previous configure.
- Build Complex version of PETSc [using c++ compiler] (add the option --with-fortran-kernels=generic to get possibly faster complex number performance on some systems):

henry@bluebottle:"/Desktop/PETSC/petsc-3.5.3\$./configure --with-cc=gcc --with-fc=gfortran --with-cxx=g++ --with-clanguage=cxx --download-fblaslapack --download-mpich --with-scalar-type=complex

Note that --with-clanguage=cxx means that the PETSc source code is compiled with the C++ compiler. This is not normally needed and we don't recommend it. One can use 'c' build of PETSc from both C and C++. One can also have a complex build with C99.

- Install 2 variants of PETSc. Specify different PETSC\_ARCH for each build.
  - With gnu

henry@bluebottle:"/Desktop/PETSC/petsc-3.5.3\$./configure PETSC\_ARCH=linux-gnu --with-cc=gcc --with-cxx=g++ --with-fc=gfortran --download-mpichhenry@bluebottle:"/Desktop/PETSC/petsc-3.5.3\$make PETSC\_ARCH=linux-gnu all test

- With intel compilers (intel use mkl instead of blas and lapack).

henry@bluebottle:"/Desktop/PETSC/petsc-3.5.3\$./configure PETSC\_ARCH=linux-gnu-intel --with-cc=icc --with-ccx=icpc --with-fc=ifort --download-mpich --with-blas-lapack-dir=/usr/local/mklhenry@bluebottle:"/Desktop/PETSC/petsc-3.5.3\$make PETSC\_ARCH=linux-gnu-intel all test

- BLAS/LAPACK: These packages provide some basic numeric kernels used by PETSc.
  - \* Configure will automatically look for blas/lapack in certain standard locations, on most systems you should not need to provide any information about BLAS/LAPACK in the ./configure command.
  - \* One can use the following options to let configure download/install blas/lapack automatically.
    - · --download-fblaslapack [when fortran compiler is present]
    - · --download-f2cblaslapack [when configuring without a fortran compiler i.e --with-fc=0]
  - \* Alternatively one can use other options like one of the following.
    - · --with-blas-lapack-lib=libsunperf.a
    - · --with-blas-lib=libblas.a --with-lapack-lib=liblapack.a
    - · --with-blas-lapack-dir=/soft/com/packages/intel/13/079/mkl
- Specify environment variable for bash [can be specified in ~/.bashrc]

```
export PETSC_DIR=~/Desktop/PETSC/petsc-3.5.3
export PETSC_ARCH=linux-gnu-c-debug
```

# 10 Find out if compiler names are within the \$PATH

If this is the case. No need for explicit specification on the configuration.

```
henry@bluebottle:~/Desktop$ which gcc
/usr/bin/gcc
henry@bluebottle:~/Desktop$ which g++
/usr/bin/g++
henry@bluebottle:~/Desktop$ which gfortran
/usr/bin/gfortran
henry@bluebottle:~/Desktop$ which mpicc
/usr/bin/mpicc
henry@bluebottle:~/Desktop$ which mpicxx
/usr/bin/mpicxx
henry@bluebottle:~/Desktop$ which mpif90
/usr/bin/mpif90
```

### 11 FFTW

--download-PACKAGENAME=/PATH/TO/package.tar.gz: If ./configure cannot automatically download the package [due to network/firewall issues], one can download the package by alternaive means [perhaps wget or scp via some other machine]. Once the tarfile is downloaded, the path to this file can be specified to configure with this option. Configure will proceed to install this package and then configure PETSc with it.

Since FFTW need to configure for a MPI. We download fftw and set the \$PATH to be install it.

--download-fftw=/home/henry/Desktop/FFTW/downloads\_fftw/fftw-3.5.3.tar.gz

### 12 Install PETSC Manually

henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3\$ 11

### 12.1 Before you start your installation

You made want to know how your petsc folder look like because it is going to change a little.

```
total 8756
drwxr-xr-x 12 henry henry
                             4096 May 23 17:42 ./
drwxrwxr-x 7 henry henry
                             4096 Aug 10 10:57 ../
drwxr-xr-x
           6 henry henry
                             4096 May 23 17:42 bin/
drwxr-xr-x
           2 henry henry
                             4096 May 23 17:42 conf/
drwxr-xr-x 5 henry henry
                            4096 May 23 17:42 config/
                             340 Sep 8
                                        2014 configure
-rwxr-xr-x 1 henry henry
-rw-r--r--
                            1751 Sep 8 2014 CONTRIBUTING
           1 henry henry
-rw-r--r--
           1 henry henry 6336652 May 23 17:42 CTAGS
-rw-r--r-- 1 henry henry
                            6844 Sep 8 2014 .dir-locals.el
                            4096 May 23 17:42 docs/
drwxr-xr-x 4 henry henry
-rw-r--r--
                            8798 May 23 10:57 gmakefile
           1 henry henry
drwxr-xr-x 6 henry henry
                            4096 May 23 17:42 include/
-rw-r--r--
           1 henry henry
                             815 May 23 17:42 index.html
                            4096 May 23 17:42 interfaces/
drwxr-xr-x 3 henry henry
-rw-r--r--
                            1526 Sep 8 2014 LICENSE
           1 henry henry
-rw-r--r--
                           27891 May 23 17:42 makefile
             henry henry
           1
-rw-r--r--
                           34168 May 23 17:42 makefile.html
           1 henry henry
-rwxr-xr-x 1 henry henry
                            9775 Jan 30 2015 setup.py*
                            4096 May 13
drwxr-xr-x 3 henry henry
                                         2013 share/
drwxr-xr-x 12 henry henry
                            4096 May 23 17:42 src/
drwxr-xr-x 3 henry henry
                            4096 May 13 2013 systems/
           1 henry henry 2458233 May 23 17:42 TAGS
drwxr-xr-x 3 henry henry
                            4096 May 23 17:42 tutorials/
Let's start with the installation
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ export PETSC_DIR=~/Desktop/PETSC/petsc-3.5.3
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ export PETSC_ARCH=linux-gnu-complex
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ ./configure
            Configuring PETSc to compile on your system
TESTING: alternateConfigureLibrary from PETSc.packages.mpi4py(config/PETSc/packages/mpi4py.py:56)
Compilers:
                     mpicc -fPIC -Wall -Wwrite-strings -Wno-strict-aliasing -Wno-unknown-pragmas -g3 -00
  C Compiler:
                     mpicxx -Wall -Wwrite-strings -Wno-strict-aliasing -Wno-unknown-pragmas -g -00 -fPIC
  C++ Compiler:
  Fortran Compiler: mpif90 -fPIC -Wall -Wno-unused-variable -ffree-line-length-0 -Wno-unused-dummy-argument -g -00
```

```
Linkers:
  Shared linker: mpicc -shared -fPIC -Wall -Wwrite-strings -Wno-strict-aliasing -Wno-unknown-pragmas -g3 -00
  Dynamic linker: mpicc -shared -fPIC -Wall -Wwrite-strings -Wno-strict-aliasing -Wno-unknown-pragmas -g3 -00
make:
MPI:
 Includes: -I/usr/lib/openmpi/include -I/usr/lib/openmpi/include/openmpi
BLAS/LAPACK: -llapack -lblas
X:total 21312
drwxr-xr-x 14 henry henry
                              4096 Apr 27 13:43 ./
                              4096 May 1 13:28 ../
4096 Apr 24 10:40 bin/
drwxrwxr-x 6 henry henry
drwxr-xr-x 6 henry henry
                             62332 Apr 27 13:40 CMakeLists.txt
           1 henry henry
                              4096 Apr 24 10:40 conf/
drwxr-xr-x 2 henry henry
                              4096 Apr 24 10:40 config/
drwxr-xr-x 5 henry henry
-rwxr-xr-x 1 henry henry
                              340 Sep 8 2014 configure*
                                28 Apr 27 13:40 configure.log -> linux-dbg/conf/configure.log
lrwxrwxrwx 1 henry henry
                                32 Apr 27 13:40 configure.log.bkp -> linux-dbg/conf/configure.log.bkp
lrwxrwxrwx 1 henry henry
-rw-rw-r--
           1 henry henry
                           1963859 Apr 24 23:03 configure_log.txt
-rw-r--r-- 1 henry henry
                              1751 Sep 8 2014 CONTRIBUTING
-rw-r--r- 1 henry henry
                           6330591 Jan 31 00:14 CTAGS
drwxrwxr-x 6 henry henry
                              4096 Apr 24 10:40 -dbg/
-rw-r--r-- 1 henry henry
                              6844 Sep 8 2014 .dir-locals.el
drwxr-xr-x 4 henry henry
                              4096 Jan 31 00:14 docs/
-rw-r--r-- 1 henry henry
                              8681 Sep 8 2014 gmakefile
drwxr-xr-x 6 henry henry
                              4096 Jan 31 00:14 include/
-rw-r--r-- 1 henry henry
                              816 Jan 31 00:14 index.html
drwxr-xr-x 3 henry henry
                              4096 Jan 31 00:14 interfaces/
-rw-r--r- 1 henry henry
                              1526 Sep 8 2014 LICENSE
drwxrwxr-x 7 henry henry
                              4096 Apr 25 19:45 linux-dbg/
                             27795 Jan 31 00:14 makefile
-rw-r--r-- 1 henry henry
-rw-r--r-- 1 henry henry
                             34073 Jan 31 00:14 makefile.html
lrwxrwxrwx 1 henry henry
                                23 Apr 27 13:40 make.log -> linux-dbg/conf/make.log
                                0 Apr 28 18:52 .nagged
-rw-rw-r-- 1 henry henry
-rw-rw-r-- 1 henry henry 10825568 Apr 27 13:40 RDict.log
                              9775 Jan 30 23:23 setup.py*
-rwxr-xr-x 1 henry henry
drwxr-xr-x 3 henry henry
                              4096 May 13 2013 share/
drwxr-xr-x 12 henry henry
                              4096 Jan 31 00:14 src/
                              4096 May 13 2013 systems/
drwxr-xr-x 3 henry henry
-rw-r--r- 1 henry henry 2454792 Jan 31 00:14 TAGS
drwxr-xr-x 3 henry henry
                              4096 Jan 31 00:14 tutorials/
  Library: -1X11
  Arch:
pthread:
 Library: -lpthread
ssl:
 Library: -lssl -lcrypto
valgrind:
PETSc:
  PETSC_ARCH: linux-dbg
  PETSC_DIR: /home/henry/Desktop/PETSC/petsc-3.5.3
  Clanguage: C
  shared libraries: enabled
  Scalar type: real
  Precision: double
  Memory alignment: 16
 Configure stage complete. Now build PETSc libraries with (gnumake build):
  make PETSC_DIR=/home/henry/Desktop/PETSC/petsc-3.5.3 PETSC_ARCH=linux-dbg all
Creat the object files
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ make
          CC linux-dbg/obj/src/tao/interface/taosolver_bounds.o
          CC linux-dbg/obj/src/tao/interface/dlregistao.o
          CC linux-dbg/obj/src/tao/interface/fdiff.o
          CC linux-dbg/obj/src/tao/interface/fdtest.o
          CC linux-dbg/obj/src/tao/interface/ftn-auto/taosolver_boundsf.o
          CC linux-dbg/obj/src/tao/interface/ftn-auto/taosolver_fgf.o
          CC linux-dbg/obj/src/tao/interface/ftn-auto/taosolver_hjf.o
          CC linux-dbg/obj/src/tao/interface/ftn-auto/taosolverf.o
          CC linux-dbg/obj/src/tao/interface/ftn-custom/ztaosolverf.o
          CC linux-dbg/obj/src/tao/unconstrained/impls/nls/nls.o
          CC linux-dbg/obj/src/tao/unconstrained/impls/neldermead/neldermead.o
          CC linux-dbg/obj/src/tao/unconstrained/impls/ntr/ntr.o
          CC linux-dbg/obj/src/tao/unconstrained/impls/cg/taocg.o
          CC linux-dbg/obj/src/tao/unconstrained/impls/lmvm/lmvm.o
```

```
CC linux-dbg/obj/src/tao/unconstrained/impls/bmrm/bmrm.o
          CC linux-dbg/obj/src/tao/unconstrained/impls/ntl/ntl.o
          CC linux-dbg/obj/src/tao/unconstrained/impls/owlan/owlan.o
          CC linux-dbg/obj/src/tao/constrained/impls/ipm/ipm.o
          CC linux-dbg/obj/src/tao/linesearch/interface/taolinesearch.o
          CC linux-dbg/obj/src/tao/linesearch/interface/dlregis_taolinesearch.o
          CC linux-dbg/obj/src/tao/linesearch/interface/ftn-auto/taolinesearchf.o
          CC linux-dbg/obj/src/tao/linesearch/interface/ftn-custom/ztaolinesearchf.o
          CC linux-dbg/obj/src/tao/linesearch/impls/armijo/armijo.o
          CC linux-dbg/obj/src/tao/linesearch/impls/morethuente/morethuente.o
          CC linux-dbg/obj/src/tao/linesearch/impls/owarmijo/owarmijo.o
          CC linux-dbg/obj/src/tao/linesearch/impls/unit/unit.o
          CC linux-dbg/obj/src/tao/linesearch/impls/gpcglinesearch/gpcglinesearch.o
          CC linux-dbg/obj/src/tao/leastsquares/impls/pounders/pounders.o
          CC linux-dbg/obj/src/tao/leastsquares/impls/pounders/gqt.o
    CLINKER /home/henry/Desktop/PETSC/petsc-3.5.3/linux-dbg/lib/libpetsc.so.3.5.3
make[2]: Leaving directory '/home/henry/Desktop/PETSC/petsc-3.5.3'
make[1]: Leaving directory '/home/henry/Desktop/PETSC/petsc-3.5.3'
Now to check if the libraries are working do:
make PETSC_DIR=/home/henry/Desktop/PETSC/petsc-3.5.3 PETSC_ARCH=linux-dbg test
```

#### 12.2 A new Folder is create

Folder linux-dbg is created

```
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ 11
total 21312
drwxr-xr-x 14 henry henry
                             4096 Apr 27 13:40 ./
drwxrwxr-x 5 henry henry
                              4096 Apr 24 18:20 ../
drwxr-xr-x 6 henry henry
                             4096 Apr 24 10:40 bin/
           1 henry henry
                             62332 Apr 27 13:40 CMakeLists.txt
drwxr-xr-x 2 henry henry
                              4096 Apr 24 10:40 conf/
                              4096 Apr 24 10:40 config/
drwxr-xr-x 5 henry henry
                              340 Sep 8 2014 configure*
-rwxr-xr-x 1 henry henry
                               28 Apr 27 13:40 configure.log -> linux-dbg/conf/configure.log
lrwxrwxrwx 1 henry henry
lrwxrwxrwx 1 henry henry
                                32 Apr 27 13:40 configure.log.bkp -> linux-dbg/conf/configure.log.bkp
-rw-rw-r-- 1 henry henry
                           1963859 Apr 24 23:03 configure_log.txt
-rw-r--r-- 1 henry henry
                             1751 Sep 8 2014 CONTRIBUTING
-rw-r--r- 1 henry henry
                           6330591 Jan 31 00:14 CTAGS
drwxrwxr-x 6 henry henry
                              4096 Apr 24 10:40 -dbg/
-rw-r--r-- 1 henry henry
                              6844 Sep 8 2014 .dir-locals.el
                              4096 Jan 31 00:14 docs/
drwxr-xr-x 4 henry henry
-rw-r--r-- 1 henry henry
                              8681 Sep 8 2014 gmakefile
                              4096 Jan 31 00:14 include/
drwxr-xr-x 6 henry henry
-rw-r--r- 1 henry henry
                              816 Jan 31 00:14 index.html
drwxr-xr-x 3 henry henry
                              4096 Jan 31 00:14 interfaces/
-rw-r--r- 1 henry henry
                             1526 Sep 8 2014 LICENSE
                             4096 Apr 25 19:45 linux-dbg/
drwxrwxr-x 7 henry henry
                             27795 Jan 31 00:14 makefile
-rw-r--r-- 1 henry henry
-rw-r--r-- 1 henry henry
                             34073 Jan 31 00:14 makefile.html
                               23 Apr 27 13:40 make.log -> linux-dbg/conf/make.log
lrwxrwxrwx 1 henry henry
-rw-rw-r--
                                0 Apr 27 13:31 .nagged
           1 henry henry
-rw-rw-r--
             henry henry 10825568 Apr 27 13:40 RDict.log
                             9775 Jan 30 23:23 setup.py
-rwxr-xr-x 1 henry henry
                              4096 May 13 2013 share/
drwxr-xr-x 3 henry henry
                             4096 Jan 31 00:14 src/
drwxr-xr-x 12 henry henry
                             4096 May 13 2013 systems/
drwxr-xr-x 3 henry henry
-rw-r--r--
                          2454792 Jan 31 00:14 TAGS
           1 henry henry
drwxr-xr-x 3 henry henry
                             4096 Jan 31 00:14 tutorials/
```

#### 12.3 Now to check if the libraries are working

Now to evaluate the computer systems you plan use-do:

```
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ make PETSC_DIR=/home/henry/Desktop/PETSC/petsc-3.5.3 PETSC_ARCH=linux-dbg streams NPMAX=4
cd src/benchmarks/streams; /usr/bin/make --no-print-directory streams
mpicc -o MPIVersion.o -c -fPIC -Wall -Wwrite-strings -Wno-strict-aliasing -Wno-unknown-pragmas -g3 -00
                                                                                                          -I/home/henry/Desktop/PETSC/petsc-3.5.3/include
/home/henry/Desktop/PETSC/petsc-3.5.3/src/benchmarks/streams/MPIVersion.c: In function main:
/home/henry/Desktop/PETSC/petsc-3.5.3/src/benchmarks/streams/MPIVersion.c:99:7: warning: value computed is not used [-Wunused-value]
/home/henry/Desktop/PETSC/petsc-3.5.3/src/benchmarks/streams/MPIVersion.c:103:4: warning: value computed is not used [-Wunused-value]
Number of MPI processes 1
Process 0 bluebottle
              Rate (MB/s)
Function
            11785.8911
Copy:
            11347.4576
Scale:
            13004.7537
Add:
Triad:
            12298.5090
Number of MPI processes 2
Process 0 bluebottle
Process 1 bluebottle
             Rate (MB/s)
Function
            12171.7356
Scale:
            12082.4353
Add:
            13361.2045
Triad:
            13562.3699
Number of MPI processes 3
Process 0 bluebottle
Process 1 bluebottle
Process 2 bluebottle
Function
              Rate (MB/s)
Copy:
            12192.0058
Scale:
            12130.3003
Add:
            13479.2845
Triad:
            13570.7497
Number of MPI processes 4
Process 0 bluebottle
Process 1 bluebottle
Process 2 bluebottle
Process 3 bluebottle
              Rate (MB/s)
{\tt Function}
Copy:
            12592.1116
Scale:
            12085.5584
Add:
            13892.1390
Triad:
            13938.5530
np speedup
1 1.0
2 1.1
3 1.1
4 1.13
Estimation of possible speedup of MPI programs based on Streams benchmark.
It appears you have 1 node(s)
See graph in the file src/benchmarks/streams/scaling.png
              scaling-eps-converted-to.pdf
```

PetscScalar: Evaluate the Computer System using Real Numbers

### 13 Complex Configuration

```
henry@bluebottle:~/Desktop/PETSC$ cd petsc-3.5.3/
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ export PETSC_DIR=~/Desktop/PETSC/petsc-3.5.3
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ export PETSC_ARCH=linux-dbg-Complex
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ ./configure --with-cc=gcc --with-fc=gfortran --with-cxx=g++ --with-clanguage=cxx
  -download-fblaslapack --download-mpich --with-scalar-type=complex
                           Configuring PETSc to compile on your system
                                              /home/henry/Desktop/PETSC/petsc-3.5.3/linux-dbg-Complex/bin/mpicc -fPIC -Wall -Wwrite-strings -Wno-strict-aliasing -Wno-unknown-pragmatic -Wno-strict-aliasing -Wno-unknown-pragmatic -Wno-strict-aliasing -Wno-unknown-pragmatic -Wno-strict-aliasing -Wno-strict-
   C Compiler:
   C++ Compiler:
                                             Fortran Compiler:
Linkers:
   \label{linker: Shared linker: Shar
make:
   Includes: -I/home/henry/Desktop/PETSC/petsc-3.5.3/linux-dbg-Complex/include
BLAS/LAPACK: -W1,-rpath,/home/henry/Desktop/PETSC/petsc-3.5.3/linux-dbg-Complex/lib -L/home/henry/Desktop/PETSC/petsc-3.5.3/linux-dbg-Complex/lib -lfla
fblaslapack:
   Library: -1X11
   Arch:
pthread:
   Library: -lpthread
ssl:
   Library: -lssl -lcrypto
valgrind:
PETSc:
   PETSC_ARCH: linux-dbg-Complex
   PETSC_DIR: /home/henry/Desktop/PETSC/petsc-3.5.3
   Clanguage: Cxx
   shared libraries: enabled
   Scalar type: complex
   Precision: double
   Memory alignment: 16
  Configure stage complete. Now build PETSc libraries with (gnumake build):
      make PETSC_DIR=/home/henry/Desktop/PETSC/petsc-3.5.3 PETSC_ARCH=linux-dbg-Complex all
Creat the objects Files
 henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ make
                  CXX linux-dbg-Complex/obj/src/ts/impls/implicit/theta/theta.o
                   {\tt CXX\ linux-dbg-Complex/obj/src/ts/impls/implicit/theta/ftn-auto/thetaf.o}
                   CXX linux-dbg-Complex/obj/src/ts/impls/implicit/alpha/alpha.o
                  {\tt CXX\ linux-dbg-Complex/obj/src/ts/impls/implicit/alpha/ftn-auto/alphaf.o}
                  CXX linux-dbg-Complex/obj/src/ts/interface/ts.o
                  CXX linux-dbg-Complex/obj/src/ts/interface/tscreate.o
                   CXX linux-dbg-Complex/obj/src/ts/interface/tsreg.o
                  CXX linux-dbg-Complex/obj/src/ts/interface/tsregall.o
                  CXX linux-dbg-Complex/obj/src/ts/interface/dlregists.o
                  CXX linux-dbg-Complex/obj/src/ts/interface/tseig.o
                   CXX linux-dbg-Complex/obj/src/ts/interface/ftn-auto/tsf.o
                  CXX linux-dbg-Complex/obj/src/ts/interface/ftn-custom/ztscreatef.o
                   {\tt CXX\ linux-dbg-Complex/obj/src/ts/interface/ftn-custom/ztsf.o}
                  CXX linux-dbg-Complex/obj/src/ts/interface/ftn-custom/ztsregf.o
                   CXX linux-dbg-Complex/obj/src/ts/adapt/interface/tsadapt.o
                   CXX linux-dbg-Complex/obj/src/ts/adapt/interface/ftn-auto/tsadaptf.o
                   CXX linux-dbg-Complex/obj/src/ts/adapt/impls/cfl/adaptcfl.o
                   CXX linux-dbg-Complex/obj/src/ts/adapt/impls/none/adaptnone.o
                   CXX linux-dbg-Complex/obj/src/ts/adapt/impls/basic/adaptbasic.o
                    FC linux-dbg-Complex/obj/src/ts/f90-mod/petsctsmod.o
                   CXX linux-dbg-Complex/obj/src/tao/matrix/lmvmmat.o
                   CXX linux-dbg-Complex/obj/src/tao/matrix/adamat.o
                   CXX linux-dbg-Complex/obj/src/tao/matrix/submatfree.o
                   CXX linux-dbg-Complex/obj/src/tao/util/tao_util.o
                   CXX linux-dbg-Complex/obj/src/tao/util/ftn-auto/tao_utilf.o
                   CXX linux-dbg-Complex/obj/src/tao/interface/taosolver.o
                   CXX linux-dbg-Complex/obj/src/tao/interface/taosolver_fg.o
                   CXX linux-dbg-Complex/obj/src/tao/interface/taosolverregi.o
```

CXX linux-dbg-Complex/obj/src/tao/interface/taosolver\_hj.o

```
CXX linux-dbg-Complex/obj/src/tao/interface/taosolver_bounds.o
         CXX linux-dbg-Complex/obj/src/tao/interface/dlregistao.o
         CXX linux-dbg-Complex/obj/src/tao/interface/fdiff.o
         CXX linux-dbg-Complex/obj/src/tao/interface/fdtest.o
         CXX linux-dbg-Complex/obj/src/tao/interface/ftn-auto/taosolver_boundsf.o
         CXX linux-dbg-Complex/obj/src/tao/interface/ftn-auto/taosolver_fgf.o
         CXX linux-dbg-Complex/obj/src/tao/interface/ftn-auto/taosolver_hjf.o
         CXX linux-dbg-Complex/obj/src/tao/interface/ftn-auto/taosolverf.o
         CXX linux-dbg-Complex/obj/src/tao/interface/ftn-custom/ztaosolverf.o
         CXX linux-dbg-Complex/obj/src/tao/linesearch/interface/taolinesearch.o
         CXX linux-dbg-Complex/obj/src/tao/linesearch/interface/dlregis_taolinesearch.o
         {\tt CXX\ linux-dbg-Complex/obj/src/tao/linesearch/interface/ftn-auto/taolinesearchf.ode}
         {\tt CXX\ linux-dbg-Complex/obj/src/tao/linesearch/interface/ftn-custom/ztaolinesearchf.ode}
     {\tt CLINKER~/home/henry/Desktop/PETSC/petsc-3.5.3/linux-dbg-Complex/lib/libpetsc.so.3.5.3}
make[2]: Leaving directory '/home/henry/Desktop/PETSC/petsc-3.5.3'
make[1]: Leaving directory '/home/henry/Desktop/PETSC/petsc-3.5.3'
Now to check if the libraries are working do:
make PETSC_DIR=/home/henry/Desktop/PETSC/petsc-3.5.3 PETSC_ARCH=linux-dbg-Complex test
Check if the library are working
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ make PETSC_DIR=/home/henry/Desktop/PETSC/petsc-3.5.3 PETSC_ARCH=linux-dbg-Complex test
Running test examples to verify correct installation
Using PETSC_DIR=/home/henry/Desktop/PETSC/petsc-3.5.3 and PETSC_ARCH=linux-dbg-Complex
C/C++ example src/snes/examples/tutorials/ex19 run successfully with 1 MPI process
C/C++ example src/snes/examples/tutorials/ex19 run successfully with 2 MPI processes
Fortran example src/snes/examples/tutorials/ex5f run successfully with 1 MPI process
Completed test examples
Now to evaluate the computer systems you plan use - do:
make PETSC_DIR=/home/henry/Desktop/PETSC/petsc-3.5.3 PETSC_ARCH=linux-dbg-Complex streams NPMAX=<number of MPI processes you intend to use>
Now we evaluate the computer system you plan to use:
henry@bluebottle:~/Desktop/PETSC/petsc-3.5.3$ make PETSC_DIR=/home/henry/Desktop/PETSC/petsc-3.5.3 PETSC_ARCH=linux-dbg-Complex streams NPMAX=4
cd src/benchmarks/streams; /usr/bin/make --no-print-directory streams
/home/henry/Desktop/PETSC/petsc-3.5.3/linux-dbg-Complex/bin/mpicxx -o MPIVersion.o -c -Wall -Wwrite-strings -Wno-strict-aliasing -Wno-unknown-pragmas -
Number of MPI processes 1
Process 0 bluebottle
             Rate (MB/s)
Function
            11076.8118
Copy:
            10638.6912
Scale:
Add:
            12522.6468
Triad:
            12336.1882
Number of MPI processes 2
Process 0 bluebottle
Process 1 bluebottle
Function
             Rate (MB/s)
            12778.3848
Copy:
Scale:
            12660.8554
Add:
           14196.9249
Triad:
            14360.4703
Number of MPI processes 3
Process 0 bluebottle
Process 1 bluebottle
Process 2 bluebottle
Function
             Rate (MB/s)
            12539.6763
Copy:
            12434,2251
Scale:
            13975.9454
Add:
           14031.1417
Triad:
Number of MPI processes 4
Process 0 bluebottle
Process 1 bluebottle
Process 2 bluebottle
Process 3 bluebottle
              Rate (MB/s)
Function
            12412.4117
Copy:
            12379,4968
Scale:
Add:
            13801.3317
Triad:
           13867.5576
np speedup
1 1.0
2 1.16
3 1.14
4 1.12
Estimation of possible speedup of MPI programs based on Streams benchmark.
It appears you have 1 node(s)
See graph in the file src/benchmarks/streams/scaling.png
```



PetscScalar: Evaluate the Computer System using Complex Numbers

### 14 Use BASH file to untar, install and configure

```
#!/bin/bash
henry@bluebottle:~$ tar zxvf /Desktop/PETSC/petsc-3.5.3.tar.gz # untar petsc on a particular folder
cd Desktop/PETSC/petsc-3.5.3 # move to petsc folder
export PETSC_DIR=~/Desktop/PETSC/petsc-3.5.3
export PETSC_ARCH=linux-gnu-complex
./configure PETSC_ARCH=linux-gnu-complex --with-scalar-type=complex --download-fftw --with-debugging=1
make
make all test # In one step:

In two steps:
make all
make test
On this configure.
```

On this configuration:

- PETSC\_ARCH=linux-gnu-complex give a name to configuration/build
- Complex number configuration is using: --with-scalar-type=complex
- If BLAS, LAPACK, MPI are install already. The default system/compiler locations are availab via PATH. No need for these:

```
--with-blas-lapack-dir=/usr/local/blaslapack
--with-mpi-dir=/usr/local/mpich
--with-cc=mpicc --with-cxx=mpicxx --with-fc=mpif90
```

• fftw is install but it is not setup for mpi. We hope the download of fftw will configure fftw for mpi, No need to include the PATH to fftw: --with-fftw-dir=/usr/include/

## 15 Compile and Execute Hello World Example

#### 15.1 On my Desktop PC

My Hello world c code: example\_hello\_0\_C.c

```
#include <petsc.h>
int main ( int argc, char *argv[] ){
   PetscErrorCode ierr;
  PetscMPIInt
                 rank. size:
  PetscInitialize(&argc, &argv, PETSC_NULL,PETSC_NULL);
ierr = MPI_Comm_size(PETSC_COMM_WORLD,&size);
  CHKERRQ(ierr); /* Checks error code, if non-zero it calls the error handler and then returns */
   ierr = MPI_Comm_rank(PETSC_COMM_WORLD,&rank);
  CHKERRQ(ierr);
/* Prints to standard out, only from the first processor in the communicator. Calls from other processes are ignored.
  Specifically designed to print the message once for all the processes */
   // \texttt{PetscPrintf(PETSC\_COMM\_WORLD,"Number of processors = \%d, rank = \%d\n", size, rank);}
   //PetscPrintf(PETSC_COMM_WORLD, "Hello World from [%d] rank\n",rank);
/* Prints to standard out, from all processor in the communicator. Specifically designed to print the message from each of the processes*/
  PetscPrintf(PETSC_COMM_SELF,"Hello World from [%d] rank\n",rank);
PetscPrintf(PETSC_COMM_SELF,"Number of processors = %d, rank = %d\n",size,rank);
  PetscFinalize();
   return 0;
Makefile file: Makefile
CFLAGS
FFLAGS
CPPFLAGS
FPPFLAGS
LOCDIR
                 = home/Desktop/PETSC/Examples/example_0/
EXAMPLESC
                 = example_hello_0_C.c example_hello_1_C.c
EXAMPLESF
                 = example_hello_0_F.f
                 = example_0
include ${PETSC_DIR}/conf/variables
include ${PETSC_DIR}/conf/rules
example_hello_0_C: example_hello_0_C.o chkopts
-${CLINKER} -o out example_hello_0_C.o ${PETSC_LIB}
${RM} example_hello_0_C.o
example_hello_1_C: example_hello_1_C.o chkopts
-${CLINKER} -o out example_hello_1_C.o ${PETSC_LIB}
${RM} example_hello_1_C.o
example_hello_0_F: example_hello_0_F.o chkopts
-${CLINKER} -o example_hello_0_F example_hello_0_F.o ${PETSC_LIB}
${RM} example_hello_0_F.o
Bash file: compile_and_execute.sh
#!/bin/bash
export PETSC_DIR=~/Desktop/PETSC/petsc-3.5.3
export PETSC_ARCH=linux-dbg
make example_hello_0_C
mpirun -np 4 out
Compile with using just the makefile
henry@bluebottle:~/Desktop/PETSC/Examples/example_0$ export PETSC_DIR=~/Desktop/PETSC/petsc-3.5.3
henry@bluebottle:~/Desktop/PETSC/Examples/example_0$ make example_hello_0_C
mpicc -fPIC -Wall -Wwrite-strings -Wno-strict-aliasing -Wno-unknown-pragmas -g3 -00 -o example_hello_0_C example_hello_0_C.o -Wl,-rpath,/home/henry/Do
lutil -lgcc_s -lpthread -ldl
/bin/rm -f example_hello_0_C.o
Execute Hello example
henry@bluebottle:~/Desktop/PETSC/Examples/example_0$ mpirun -np 4 example_hello_0_C
/bin/rm -f example_hello_0_C.o
Hello World from [0] rank
Number of processors = 4, rank = 0
Hello World from [1] rank
Number of processors = 4, rank = 1
Hello World from [2] rank
Number of processors = 4, rank = 2
Hello World from [3] rank
Number of processors = 4, rank = 3
```

Compile and Execute using a bash file on my Desktop. Maybe you will need to change the permission of your bash

```
henry@bluebottle:~/Desktop/PETSC/Examples/example_0$ ./compile_and_execute.sh
bash: ./compile_and_execute.sh: Permission denied
henry@bluebottle:~/Desktop/PETSC/Examples/example_0$ chmod 777 compile_and_execute.sh
henry@bluebottle:~/Desktop/PETSC/Examples/example_0$ ./compile_and_execute.sh
```

#### 15.2 On STAMPEDE

Since petsc is already installe and compile on Stapede. We just need to check how we can submit a job. of cource always is easy to start with a small program

```
example_hello_0_C.c
     #include <petsc.h>
     int main ( int argc, char *argv[] ){
        PetscErrorCode ierr;
        PetscMPIInt
                       rank, size;
        PetscInitialize(&argc, &argv, PETSC_NULL,PETSC_NULL);
        ierr = MPI_Comm_size(PETSC_COMM_WORLD,&size);
        CHKERRQ(ierr); /* Checks error code, if non-zero it calls the error handler and then returns */
        ierr = MPI_Comm_rank(PETSC_COMM_WORLD,&rank);
        CHKERRQ(ierr);
     /* Prints to standard out, only from the first processor in the communicator. Calls from other processes
     are ignored. Specifically designed to print the message once for all the processes \ast /
         //PetscPrintf(PETSC_COMM_WORLD,"Number of processors = %d, rank = %d\n",size,rank);
         //PetscPrintf(PETSC_COMM_WORLD, "Hello World from [%d] rank\n",rank);
     /* Prints to standard out, from all processor in the communicator. Specifically designed to print the message from each of the processes*/
        PetscPrintf(PETSC_COMM_SELF, "Hello World from [%d] rank\n", rank);
        \label{lem:petscPrintf} PetscPrintf(PETSC\_COMM\_SELF,"Number of processors = \mbox{\em d}, rank = \mbox{\em d} \mbox{\em n}, size, rank);
        PetscFinalize():
        return 0;
Makefile
     CFLAGS
     FFLAGS
     CPPFLAGS
     FPPFLAGS
                       = /home1/02817/hmoncada/CPS_5310/example_1
     LOCDIR
     EXAMPLESC
                       = example_hello_0_C.c example_hello_1_C.c
     EXAMPLESE
     MANSEC
                       = example_1
     include ${PETSC_DIR}/conf/variables
     include ${PETSC_DIR}/conf/rules
     example_hello_0_C: example_hello_0_C.o chkopts
      -${CLINKER} -o out example_hello_0_C.o ${PETSC_LIB}
     ${RM} example_hello_0_C.o
     example_hello_1_C: example_hello_1_C.o chkopts
              -${CLINKER} -o out example_hello_1_C.o ${PETSC_LIB}
             ${RM} example_hello_1_C.o
     #!/bin/bash
```

```
#SBATCH -A TG-ASC140011
                                  # account name
#SBATCH -J example_hello_0_C
                                  # job name
                                 # output file
#SBATCH -o example_out.%j
#SBATCH -e example_err.%j
                                 # error file
#SBATCH -N 1
                                 # total nodes requested
#SBATCH -n 4
                                  # total MPI tasks requested
#SBATCH -p serial
                                  # queue name
#SBATCH -t 00:02:00
                                  # total time requested <hh:mm:ss>
```

```
module load petsc
module list
export PETSC_DIR=/opt/apps/intel13/mvapich2_1_9/petsc/3.5/
export PETSC_ARCH=sandybridge
make example_hello_0_C
ibrun ./out > log.txt
```

Compile and execute the hello example

1. Open TERMINAL 1. On your laptop or desktop open a first Terminal. Login into stampede:

```
>> ssh user_name@stampede.tacc.utexas.edu
or
>> ssh user_name@login.xsede.org
```

2. Set your workspace

```
>> mkdir CPS_3510
>> cd CPS_3510
>> mkdir example
>> cd example
```

- **3.** Open TERMINAL 2. Copy all the file on this email into the folder example. On your laptop or desktop open a second Terminal. Next, Go to the folder where you have or save this files.
  - **3.1** On that folder you call sftp

```
>> sftp user_name@stampede.tacc.utexas.edu
or
>> sftp user_name@login.xsede.org
```

**3.2** Look for the folder where you want to save this files

```
>> cd CPS_3510
>> cd example
>> put *
>> ls
>> exit
```

How to use put and get. Please see Transferring Files with SFTP below

4. ON TERMINAL 1. Compile and execute

```
>> sbatch iob
             Welcome to the Stampede Supercomputer
--> Verifying valid submit host (login4)...OK
--> Verifying valid jobname...OK
--> Enforcing max jobs per user...OK
--> Verifying availability of your home dir (/home1/02817/hmoncada)...OK
--> Verifying availability of your work dir (/work/02817/hmoncada)...OK
--> Verifying availability of your scratch dir (/scratch/02817/hmoncada)...OK
--> Verifying valid ssh keys...OK
--> Verifying access to desired queue (serial)...OK
--> Verifying job request is within current queue limits...OK
--> Checking available allocation (TG-ASC140011)...OK
Submitted batch job 5396653
check your job
>> squeue -u 5396653
            JOBID
                    PARTITION
                                   NAME
                                           USER ST
                                                         TIME NODES NODELIST (REASON)
or
>> squeue -u hmoncada
            JOBID PARTITION
                                  NAME
                                           USER ST
                                                         TIME NODES NODELIST (REASON)
           5396653
                       serial fdder_Pe hmoncada PD
                                                         0:00
                                                                   1 (Resources)
```

5. Wait for around 5 min. Next job.txt is the final output

```
>> vi job.txt
```

### 16 Transferring Files with SFTP

### 16.1 Transferring Remote Files to the Local System

If we would like download files from our remote host, we can do so by issuing the following command:

```
get remoteFile
```

```
Fetching /home/demouser/remoteFile to remoteFile /home/demouser/remoteFile 100% 37KB 36.8KB/s 00:01
```

As you can see, by default, the "get" command downloads a remote file to a file with the same name on the local file system. We can copy the remote file to a different name by specifying the name afterwards:

```
get remoteFile localFile
```

The "get" command also takes some option flags. For instance, we can copy a directory and all of its contents by specifying the recursive option:

```
get -r someDirectory
```

We can tell SFTP to maintain the appropriate permissions and access times by using the "-P" or "-p" flag:

```
get -Pr someDirectory
```

### 16.2 Transferring Local Files to the Remote System

Transferring files to the remote system is just as easily accomplished by using the appropriately named "put" command:

```
put localFile
```

```
Uploading localFile to /home/demouser/localFile localFile 100% 7607 7.4KB/s 00:00
```

The same flags that work with "get" apply to "put". So to copy an entire local directory, you can issue:

```
put -r localDirectory
```

One familiar tool that is useful when downloading and uploading files is the "df" command, which works similar to the command line version. Using this, you can check that you have enough space to complete the transfers you are interested in:

```
df -h
```

```
Size Used Avail (root) %Capacity 19.9GB 1016MB 17.9GB 18.9GB 4%
```

Please note, that there is no local variation of this command, but we can get around that by issuing the "!" command. The "!" command drops us into a local shell, where we can run any command available on our local system. We can check disk usage by typing:

```
!
df -h
```

```
Filesystem
                 Size
                                Avail Capacity
                                                  Mounted on
                         Used
/dev/disk0s2
                595Gi
                         52Gi
                                544Gi
                                           9%
devfs
                181Ki
                        181Ki
                                  OBi
                                         100%
                                                  /dev
                   OBi
                          OBi
                                  OBi
                                         100%
                                                  /net
map -hosts
map auto_home
                   OBi
                          OBi
                                  OBi
                                         100%
                                                  /home
```

Any other local command will work as expected. To return to your SFTP session, type:

exit

You should now see the SFTP prompt return.