http://www.scipy.org/Installing\_SciPy/BuildingGeneral

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# Building everything from source with gfortran on Ubuntu (Nov 2010)

These are instructions for building everything from source on a 64 bit Ubuntu system (Maverick: 10.10) on a multicore processor using the latest versions as of November 2010. Everything is installed in a user directory structure in \$HOME/local (/home/sam/local in my case). Administrator priviliges are required only in the beginning to disable CPU throttling while building ATLAS.

#### **Install required packages**

```
sudo apt-get install build-essential (dpkg-dev (>= 1.13.5)
```

Debian package development tools

• dep: <u>g++</u> (>= 4:4.4.3) The GNU C++ compiler

• dep: <u>gcc</u> (>= 4:4.4.3) The GNU C compiler

```
• dep: <u>libc6-dev</u>
Embedded GNU C Library: Development Libraries and Header Files
or <u>libc-dev</u>
```

virtual package provided by <u>libc6-dev</u>

• dep: <u>make</u> An utility for Directing compilation.

)

```
python-dev swig gfortran python-nose
```

#### **Step 1: Disable CPU Throttling**

ATLAS' timing algorithm require CPU throttling to be disabled. This disables it on the 0th core: sudo cpufreq-selector -g performance

Then disable it on each additional core. For a quad core processor, these commands will be required:

```
sudo cp /sys/devices/system/cpu/cpu0/cpufreq/scaling_governor
/sys/devices/system/cpu1/cpufreq/scaling_governor
sudo cp /sys/devices/system/cpu/cpu0/cpufreq/scaling_governor
```

```
/sys/devices/system/cpu/cpu2/cpufreq/scaling_governor
sudo cp /sys/devices/system/cpu/cpu0/cpufreq/scaling_governor
/sys/devices/system/cpu/cpu3/cpufreq/scaling_governor
```

#### Step 2: Build ATLAS(3.9.32) with complete Lapack(3.2.2)

Download lapack.tgz from netlib.org and atlas3.9.32.tar.bz2. Extract the atlas archive into a directory named ATLAS and from within it, issue these commands:

```
mkdir BUILD
cd BUILD
../configure -b 64 -Fa alg -fPIC --with-netlib-lapack-tarfile=<path to lapack.tgz>
--prefix=/home/sam/local
make
cd lib
make shared
make ptshared
cd ..
make install
```

Note that make ptshared might not work on a single core machine. Note also that the first "make" command above will take several hours to run, as ATLAS optimizes various performance parameters.

## Step 3: Build UMFPACK (5.5.0) with AMD (2.2.1), UFConfig(3.5.0) and CHOLMOD (1.7.1)

Dowload all four packages and extract them in the same directory. Edit UFconfig/UFconfig.mk to read:

```
CC = qcc
CFLAGS = -03 -fexceptions -m64 -fPIC
F77 = gfortran
F77FLAGS = -0 - m64 - fPIC
INSTALL LIB = /home/sam/local/lib
INSTALL INCLUDE = /home/sam/local/include
METIS PATH =
METIS =
CHOLMOD CONFIG = -DNPARTITION
Then issue the following commands
cd UMFPACK
make library
make install
cd ../AMD
make install
cd ../UFconfig
cp UFconfig.h /home/sam/local/include
```

#### Step 4: Build numpy(1.5.0)

Untar the archive, copy site.cfg.example to site.cfg and edit it:

```
[DEFAULT]
library_dirs = /home/sam/local/lib
include_dirs = /home/sam/local/include
```

In the same file, uncomment these lines:

```
[blas_opt]
libraries = ptf77blas, ptcblas, atlas
[lapack_opt]
libraries = lapack, ptf77blas, ptcblas, atlas
[amd]
amd_libs = amd
```

[umfpack]
umfpack\_libs = umfpack

For a single core machine, uncomment these lines:

```
[blas_opt]
libraries = f77blas, cblas, atlas
[lapack_opt]
libraries = lapack, f77blas, cblas, atlas
```

Then use the standard installation technique

```
python setup.py build
python setup.py install --prefix=/home/sam/local
```

#### Step 5: Build scipy(0.8.0)

Make sure that \$HOME/local/bin is in \$PATH (for f2py) and \$PYTHONPATH contains \$HOME/local/lib/python-2.6/site-packages (for numpy)

Do a standard install

```
python setup.py build
python setup.py install --prefix=/home/sam/local
```

Installing SciPy / BuildingGeneral

## **Building Scipy**

Table of contents

Contents

- 1. Building Scipy
  - 1. Introduction
  - 2. Python
  - 3. <u>Compilers</u>
  - 4. Linear Algebra libraries
    - 1. Building BLAS library from Netlib
    - 2. Building LAPACK library from Netlib
    - 3. <u>Further Instructions</u>

#### Introduction

The SciPy project provides two packages: NumPy (formerly known as core SciPy) and full SciPy. The NumPy package is a replacement of Numeric and should be installed before building the full SciPy package. Installing both packages is simple. In most cases simply executing

python setup.py install

in the numpy and scipy directories will install each package. The rest of this document concentrates on configuring, building, installing, or/and using various external software that Scipy can use for extra power.

Note that to avoid problems, it can be a good idea to remove the local build directory (if any) and existing Scipy installations, before building and installing a new version built from sources. Also note that the use of pip and especially easy\_install is not recommended, as these tools often have problems where the standard python setup.py install does not.

## Python

To build SciPy, Python version 2.4 or newer is required. Make sure that the Python package distutils is installed before continuing. For example, in Debian GNU/Linux, distutils is included in the python-dev package.

If while building <u>SciPy</u>, "error: pyconfig.h: No such file or directory" is encountered, ensure that Python is installed a directory that is different from its source.

## Compilers

To build any extension modules for Python, you'll need a C compiler.

Various SciPy modules use Fortran 77 libraries and some use C++, so you'll also need Fortran 77 and C++ compilers installed. The SciPy module Weave uses a C++ compiler at run time.

Note that SciPy is developed mainly using GNU compilers. Compilers from other vendors such as

Intel, Absoft, Sun, NAG, Compaq, Vast, Porland, Lahey, HP, IBM are supported in the form of community feedback.

gcc 3.x compilers are recommended. Note that code compiled by the Intel Fortran Compiler (IFC) is not binary compatible with code compiled by g77. Therefore, when using IFC, all Fortran codes used in SciPy must be compiled with IFC. This also includes the LAPACK, BLAS, and ATLAS libraries. Using GCC for compiling C code is OK. IFC version 5.0 is not supported.

To build NumPy, only a C compiler is required.

If you see an error message

```
ImportError: /usr/lib/atlas/libblas.so.3gf: undefined symbol:
_gfortran_st_write_done
```

when building <u>SciPy</u>, it means that <u>NumPy</u> picked up the wrong Fortran compiler during build (e.g. ifort). Recompile <u>NumPy</u> using:

```
python setup.py build --fcompiler=gnu95
```

or whichever is appropriate (see python setup.py build --help-fcompiler).

#### Linear Algebra libraries

Various SciPy packages do linear algebra computations using the LAPACK routines. SciPy's setup.py scripts can use number of different LAPACK library setups, including optimized LAPACK libraries such as ATLAS or the Accelerate/vecLib framework on OS X. The following notes give detailed information on how to prepare the build environment so that SciPy's setup.py scripts can use whatever LAPACK library setup one has.

NumPy does not require any external linear algebra libraries to be installed. However, if these are available, NumPy's setup script can detect them and use them for building. If you do not plan to build the full SciPy then you can skip this section.

#### **Building BLAS library from Netlib**

Download BLAS sources from Netlib, build libfblas.a library, and set environment variable BLAS:

```
mkdir -p ~/src/
cd ~/src/
wget http://www.netlib.org/blas/blas.tgz
tar xzf blas.tgz
cd BLAS
# NOTE: The selected fortran compiler must be consistent for BLAS, LAPACK, NumPy,
and SciPv.
# For GNU compiler on 32-bit systems:
                                                          # with g77
q77 -02 -fno-second-underscore -c *.f
gfortran -02 -std=legacy -fno-second-underscore -c *.f # with gfortran
# OR for GNU compiler on 64-bit systems:
g77 -03 -m64 -fno-second-underscore -fPIC -c *.f
                                                                     # with g77
gfortran -O3 -std=legacy -m64 -fno-second-underscore -fPIC -c *.f
                                                                     # with
afortran
# OR for Intel compiler:
ifort -FI -w90 -w95 -cm -03 -unroll -c *.f
```

```
# Continue below irrespective of compiler:
ar r libfblas.a *.o
ranlib libfblas.a
rm -rf *.o
export BLAS=~/src/BLAS/libfblas.a
```

See the note at the end of the section below on building LAPACK.

#### **Building LAPACK library from Netlib**

Download LAPACK sources from Netlib, build libflapack.a library, and set environment variable LAPACK:

```
mkdir -p ~/src
wget http://www.netlib.org/lapack/lapack.tgz
tar xzf lapack.tgz
cd ~/src/LAPACK
cp INSTALL/make.inc.gfortran make.inc  # on Linux with lapack-3.2.1 or
newer
cp INSTALL/make.inc.LINUX make.inc
                                              # on Linux with older lapack
# Edit make.inc as follows:
# For GNU compiler on 32-bit Linux (these are the defaults):
PLAT = \_LINUX
0PTS = -02
# OR for GNU compiler on 64-bit Linux:
PLAT = \_LINUX
OPTS = -02 - m64 - fPIC
NOOPT = -m64 - fPIC
# OR for Absoft (8.x or later):
PLAT = LINUX
OPTS = -03 - YNO CDEC
# OR for Intel Fortran compiler on Linux:
wget http://www.scipy.org/download/misc/make.inc.LINUX IFC
cp make.inc.LINUX IFC make.inc
# Continue below irrespective of compiler:
make lapacklib
make clean
cp lapack LINUX.a libflapack.a
                                               # on Linux
export LAPACK=~/src/LAPACK/libflapack.a
```

In the event that <u>SciPy</u> is unable to find the libf\* names, a symbolic link can be made from these files to libblas.a and liblapack.a. <u>NumPy</u> is not expected to have this problem.

#### **Further Instructions**

More detailed platform-specific instructions for building and installing SciPy can be found on the <u>Installing SciPy</u> page.

#### Installing SciPy / Mac OS X

Table of contents

Contents

- 1. Python
- 2. Apple's Developer Tools
- 3. <u>FORTRAN</u>
- 4. Obtaining and Building NumPy and SciPy

These instructions describe how to install <u>NumPy</u> and <u>SciPy</u> from source. If you would rather install pre-built binaries, go to the <u>Download page</u> and install the packages linked from there.

### Python

Apple ships its own version of Python with OS X. However, we *strongly* recommend installing the <u>official Python distribution</u>.

If you are missing readline support for your installation of Python, I recommend <u>following these</u> <u>instructions</u> for getting it installed with relative ease.

#### Apple's Developer Tools

Apple's Developer Tools provide a number of key libraries, particularly the <u>vecLib Framework</u>, which includes BLAS and LAPACK. Install the most recent version from <u>Apple's Developer Connection site</u> (after free registration). The most recent version may also be included on your OS X installation CD. Ensure that all components are installed by choosing **customize** when available during the install process and selecting all optional packages (at least the X11 development tools and the 10.4 SDK).

On OS X 10.6 the default gcc version is 4.2, while <u>NumPy</u> and <u>SciPy</u> need to be built with 4.0 (at least in combination with the Python from python.org). For gcc the correct version should be picked up automatically, for C++ code (only in <u>SciPy</u>) you should ensure that g++ and c++ default to 4.0. One way to achieve this is to create symlinks

\$ ln -s /usr/bin/g++-4.0 g++
\$ ln -s /usr/bin/g++-4.0 c++

and add these to the front of your PATH.

When building with Python 2.5 on OS X 10.6 it is also necessary to do

```
$ export CC=/usr/bin/gcc-4.0
```

#### FORTRAN

Though virtually any commercial C/C++ compiler may be used with <u>SciPy</u>, OS X come with GNU C compilers preinstalled. The only thing missing is the GNU FORTRAN compiler.

Binaries of gfortran (GNU F95, this is a version of the much awaited, free, open source, F95 compiler) are available from <u>this site</u> (download universal binary). We strongly recommend to use this exact

build, many other grfortran versions/builds have created problems in the past.

#### **Obtaining and Building NumPy and SciPy**

You may install <u>NumPy</u> and <u>SciPy</u> either by checking out the source files from the Git/SVN repositories, or unpacking them from a source archive file from the <u>Download page</u>. If you choose the latter, simply expand the archive (generally a gzipped tar file), otherwise check out the following branches from the repository:

\$ git clone https://github.com/numpy/numpy.git \$ svn co http://svn.scipy.org/svn/scipy/trunk scipy

Both <u>NumPy</u> and <u>SciPy</u> are built as follows:

\$ python setup.py build

\$ python setup.py install

or, using scons,

\$ python setupscons.py scons --jobs=2

The above applies to the <u>official Python distribution</u>, which is 32-bit only for 2.5/2.6/3.1 while 32/64bit bundles are available for 2.7. For alternative 64-bit Pythons (either from Apple or home-built) on Snow Leopard, you may need to extend your build flags to specify the architecture by setting LDFLAGS and FFLAGS.

Note that with distutils (setup.py) given build flags like LDFALGS do not extend but override the defaults, so you have to specify all necessary flags. Only try this if you know what you're doing! Numscons does extend the flags, so you can for example use the build command:

LDFLAGS="-arch x86\_64" FFLAGS="-arch x86\_64" python setupscons.py scons

After a successful build, you may try running the built-in unit tests for <u>SciPy</u>:

```
python
>>> import numpy
>>> numpy.test('1','10')
>>> import scipy
>>> scipy.test('1','10')
```

Be sure **not** to import numpy or scipy while you're in the numpy/scipy source tree. Change directory first.

If you have any problems installing <u>SciPy</u> on your Mac based on these instructions, please check the <u>scipy-users and scipy-dev mailing list archives</u> for possible solutions. If you are still stuck, feel free to join scipy-users for further assistance. Please have the following information ready:

- Your OS version
- The versions of gcc and gfortran and where you obtained gfortran
  - \$ gcc --version
  - \$ gfortran --version
- The versions of numpy and scipy that you are trying to install
- The full output of \$ python setup.py build

**CategoryInstallation**