Summary: Installing CFITSIO and HEALPix for Gevolution on Betzy

This document summarizes all steps used to manually download, build, and link CFITSIO and HEALPix with gevolution on the Betzy HPC system. It also includes the required Makefile changes and Slurm runtime setup.

1. Load Compiler Environment

Load the compiler and MPI toolchain modules:

```
ml purge
ml load foss/2022a GSL/2.7-GCC-11.3.0 HDF5/1.12.2-gompi-2022a
```

2. Install CFITSIO

Create a directory for local software:

```
mkdir -p $HOME/software
```

Download CFITSIO:

```
cd $HOME/software
wget https://heasarc.gsfc.nasa.gov/FTP/software/fitsio/c/cfitsio-4.4.0.tar.gz
```

Build and install CFITSIO:

```
tar -xzf cfitsio-4.4.0.tar.gz
cd cfitsio-4.4.0
./configure --prefix=$HOME/software/cfitsio
make -j8
make install
```

3. Install HEALPix (C and C++ Libraries)

Download HEALPix 3.83:

```
cd $HOME/software
wget https://downloads.sourceforge.net/project/healpix/Healpix_3.83/Healpix_3.83_2024Nov13.tar.gz
```

Extract:

```
tar -xzf Healpix_3.83_2024Nov13.tar.gz
cd Healpix_3.83
```

Configure with CFITSIO and enable C++ interface:

```
FITSDIR=$HOME/software/cfitsio ./configure --auto=cxx
```

Build HEALPix:

```
make
```

4. Gevolution Makefile Changes

Makefile header to include CFITSIO and HEALPix:

```
# programming environment

COMPILER     := mpic++

# local installs

CFITSIO_DIR  := $(HOME)/software/cfitsio

HEALPIX_DIR  := $(HOME)/software/Healpix_3.83

INCLUDE      := -I../LATfield2  -I../hiclass_new/include -I$(CFITSIO_DIR)/include
 -I$(HEALPIX_DIR)/include

LIB          := -L../hiclass_new -L$(CFITSIO_DIR)/lib -L$(HEALPIX_DIR)/lib
          -lfftw3 -lhdf5 -lgsl -lgslcblas -lmvec -lclass -lcfitsio -lchealpix -lm

HPXCXXLIB    := -lhealpix_cxx -lcxxsupport -lsharp -lcfitsio

# target and source

EXEC         := KGBevolution

SOURCE       := main.cpp

HEADERS      := $(wildcard *.hpp)

# mandatory compiler settings (LATFIELD2)

DLATFIELD2   := -DFFT3D -DHDF5

# optional compiler settings (gevolution)

DGEVOLUTION  := -DPHINONLINEAR

DGEVOLUTION  += -DBENCHMARK

DGEVOLUTION  += -DEXACT_OUTPUT_REDSHIFTS

DGEVOLUTION  += -DCOLORTERMINAL

DGEVOLUTION  += -DHAVE_HICLASS

DGEVOLUTION  += -DHAVE_HICLASS_BG

DGEVOLUTION  += -DHAVE_HEALPIX

CDBG +=

CFLAGS += $(CDBG)

# further compiler options

OPT          := -O3 -std=c++11 -w

$(EXEC): $(SOURCE) $(HEADERS) makefile
```

```
	$(COMPILER) $< -o $@ $(OPT) $(DLATFIELD2) $(DGEVOLUTION) $(INCLUDE) $(LIB
)

lccat: lccat.cpp
	$(COMPILER) $< -o $@ $(OPT) $(DGEVOLUTION) $(INCLUDE)

lcmap: lcmap.cpp
	$(COMPILER) $< -o $@ $(OPT) -fopenmp $(DGEVOLUTION) $(INCLUDE) $(LIB) $(H
PXCXXLIB)

clean:
	-rm -f $(EXEC) lccat lcmap
```

5. Slurm Job Script (Runtime Setup)

```
#!/bin/bash

#SBATCH --account=NN12015K
#SBATCH --job-name=KGB
#SBATCH --time=00:02:00
#SBATCH --nodes=4 --ntasks=16 --cpus-per-task=1
#SBATCH --output=slurm-test-%J.out
#SBATCH --mail-type=FAIL

ml load foss/2022a GSL/2.7-GCC-11.3.0 HDF5/1.12.2-gompi-2022a

export LD_LIBRARY_PATH=$HOME/software/cfitsio/lib:$HOME/software/Healpix_3.83/lib
:$LD_LIBRARY_PATH

time srun -n 16 ./KGBevolution -n 4 -m 4 -s settings.ini
```

6. Rebuild Gevolution

```
make clean
make
```