CosmoMC Installation and Running Guidelines

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CosmoMC is a Fortran 95 Markov-Chain Monte-Carlo (MCMC) engine to explore the cosmological parameter space, plus a Python suite for plotting and presenting results. This document describes the installation of the CosmoMC on a Linux system. It is written for those who want to use it in their scientific research but without much training on Linux and the program. Besides a step-by-step installation guide, we also give a brief introduction of how to run the program on both a desktop and a cluster. We share our way to generate the plots that are commonly used in the cosmological references. For more information, one can refer to the CosmoCoffee forum or contact the authors of this document. Questions and comments would be much appreciated.

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a http://cosmologist.info/cosmomc/. In this guide, we use the CosmoMC released on July 23, 2014.
b This guidebook is based on the operating system (OS) Ubuntu 14.04.1 LTS 64-bit version. For other versions of Linux, the procedures are almost the same.
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Learn, Discuss, and Contribute
For a successful installation and running of CosmoMC, the following prerequisites are required:

- **Intel@Fortran Compiler (version 13+)** ([https://software.intel.com/en-us/fortran-compilers](https://software.intel.com/en-us/fortran-compilers))
- Open MPI ([http://www.open-mpi.org](http://www.open-mpi.org))
- CFITSIO ([http://heasarc.gsfc.nasa.gov/docs/software/fitsio/fitsio.html](http://heasarc.gsfc.nasa.gov/docs/software/fitsio/fitsio.html))
- HEALPix ([http://healpix.sourceforge.net](http://healpix.sourceforge.net))
- WMAP or Planck likelihood data ([http://lambda.gsfc.nasa.gov/product/map/dr5/likelihood_get.cfm](http://lambda.gsfc.nasa.gov/product/map/dr5/likelihood_get.cfm))

The rest of the document is organized as follows. In Section I, we guide you to install the prerequisites and likelihood data that are necessary for a successful compilation of CosmoMC. In Section II, we give a brief introduction of how to run the program and the way to generate the plots that one usually sees in the references of cosmology. FAQs about running the program are also presented.

### I. INSTALLATION AND COMPILATION

**Intel@Fortran Compiler** (version 13 or a more recent release) and Open MPI are both necessary for a successful compilation of the CosmoMC package. Intel@Fortran Compiler should be installed prior to the Open MPI. Before installing these prerequisites, you need to do some presettings of your Linux system.

1. Set the password for root user.
   ```
   $ sudo passwd
   $ [sudo] password for Your_Username: (type in the password you input during the installation of the system)
   $ Enter new UNIX password: (input the new password for the root user)
   $ Retype new UNIX password: (retype the new password)
   $ password: password updated successfully
   ```
2. Run the updates before installing any new packages.
   ```
   $ sudo apt-get update
   ```
3. Have the g++ package installed.
   ```
   $ sudo apt-get install g++
   ```
4. Install the possibly essential packages you will need in your further building of other software packages.
   ```
   $ sudo apt-get install build-essential
   ```

A. Installing Intel@Fortran Compiler

CosmoMC needs Intel@Fortran Compiler (version 13 or a more recent release) to compile. Having your OS installed and preset, now we can set out to install the Intel@Fortran Compiler. A better choose is to install the **Intel@Fortran Composer XE 2013** (Intel@Fortran Compiler is a part of it.) See the following guidelines for installation [3]. My home path is `/home/limh`. All the source files are placed in the directory `/home/limh/Downloads`. All the softwares are installed into the directory `/home/limh/Programs`. My working directory is `/home/limh/workspace`. You can use your own settings during the installation.

1. Go to [https://software.intel.com/en-us/non-commercial-software-development](https://software.intel.com/en-us/non-commercial-software-development) to download a non-commercial version of Intel@Fortran Composer XE 2013 for Linux.
2. After filling a form, you will have a non-commercial serial number sent to your registered email. Use it to register and download the source file `lfcompxe_2013_sp1.3.174.tgz`.
3. Go to the Terminal and untar the file:
   ```
   $ tar -xzvf lfcompxe_2013_sp1.3.174.tgz
   ```
4. Run the `install.sh` file to start the installation. Before doing this, you may have the serial number ready.
   ```
   $ cd lfcompxe_2013_sp1.3.174
   $ ./install.sh
   ```
   Here I provide a noncommercial serial number used by myself, i.e. NTJL-484Z4TT5. It will be expired by July 19, 2015. You can then apply for another one. In the step 5 of 7, please remember to change the install directory as
(your own installing path)/intel/composer_xe_2013_sp1.3.174.

5. Set the environment variable. Enter the home directory (for me, this is /home/limh) and run:
   $ vim .bashrc

   Add the following command line at the end of the .bashrc file [4]:
   
   ```bash
   source /home/limh/Programs/intel/composer_xe_2013_sp1.3.174/bin/ifortvars.sh intel64
   ```

   For a 32-bit Linux system, use the following line instead:
   
   ```bash
   source /home/limh/Programs/intel/composer_xe_2013_sp1.3.174/bin/ifortvars.sh ia32
   ```

   (Press Esc and type in ‘:wq’ to save and exit.)

6. Restart the terminal and run:
   $ ifort --version
   ifort (IFORT) 14.0.3 20140422
   Copyright (C) 1985-2014 Intel Corporation. All right reserved.

   Seeing the above outputs means that Intel@Fortran Composer XE 2013 has already been successfully installed on your Linux. To make sure the command ifort works, please remember to run the command `source .bashrc` every time you restart the terminal.

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**B. Installing Open MPI**

After having the Intel@Fortran Compiler installed, we can set out to install the Open MPI. The installation may take almost 40 minutes.

1. Go to [http://www.open-mpi.org/software/ompi/v1.8/](http://www.open-mpi.org/software/ompi/v1.8/) to download the newest stable version. This installation is based on the Version 1.8.1.

2. Untar the source file using
   
   ```bash
   $ tar -zvxf openmpi-1.8.1.tar.gz
   ```

3. Configure and make. Do remember to set the **F77**, **FC** and **F90** environment variables before configuring (for one to use Intel@Fortran Compiler instead of Gfortran or other compilers. Here, I use a 64-bit version of Intel@Fortran Compiler), e.g.
   
   ```bash
   $ cd openmpi-1.8.1
   $ ./configure --prefix=/home/limh/Programs/openmpi F77=/home/limh/Programs/intel/composer_xe_2013_sp1.3.174/bin/intel64/ifort FC=/home/limh/Programs/intel/composer_xe_2013_sp1.3.174/bin/intel64/ifort F90=/home/limh/Programs/intel/composer_xe_2013_sp1.3.174/bin/intel64/ifort
   $ make
   $ make install
   ```

4. Go to the home directory (for me this is /home/limh) and add the following lines at the end of the .bashrc file:
   
   ```bash
   $ vi .bashrc
   ```

   Add the following line at the end of the file. Quit and save.
   ```bash
   export PATH=/home/limh/Programs/openmpi/bin:$PATH
   ```

   Then run `source .bashrc` to implement the bash settings.

   ```bash
   $ source .bashrc
   ```

5. Enter the `openmp-1.8.1/examples` directory of Open MPI to run the test.
   
   ```bash
   $ cd /scratchfs/hnlin/openmpi-1.8.1/examples
   ```

   Save and quit. Then run `make` to compile.

   ```bash
   $ make
   $ mpirun -np 4 ./hello.c
   ```

   Seeing the following outputs means that Open MPI has already been successfully installed on your Linux.

   ```plaintext
   Hello, world, I am 0 of 4, (Open MPI v1.8.1, package: Open MPI limh@limh-pc Distribution, ident: 1.8.1, Apr 22, 2014, 89)
   Hello, world, I am 1 of 4, (Open MPI v1.8.1, package: Open MPI limh@limh-pc Distribution, ident: 1.8.1, Apr 22, 2014, 89)
   Hello, world, I am 3 of 4, (Open MPI v1.8.1, package: Open MPI limh@limh-pc Distribution, ident: 1.8.1, Apr 22, 2014, 89)
   Hello, world, I am 2 of 4, (Open MPI v1.8.1, package: Open MPI limh@limh-pc Distribution, ident: 1.8.1, Apr 22, 2014, 89)
   ```
C. Installing CFITSIO

CFITSIO is also another prerequisite for one to run CosmoMC. Run the following command lines to install it.

1. Untar, configure, and make (others also use ‘make shared’ instead of ‘make’).
   
   ```
   $ tar -xzvf cfitsio3370.tar.gz
   $ cd cfitsio
   $ ./configure --prefix=/home/limh/Programs/cfitsio
   $ make
   $ make install
   ```

2. Go to the home directory (for me this is `/home/limh`) and add the following lines at the end of the `.bashrc` file:

   ```
   $ vi .bashrc
   Add the following line at the end of the file. Quit and save.
   ```
   ```
   export LD_LIBRARY_PATH=/home/limh/Programs/cfitsio/lib:$LD_LIBRARY_PATH
   ```

D. Installing HEALPix

The installation of HEALPix is a little bit bothersome. One can build the facilities with a number of compilers, i.e. C, C++, Fortran, Python, etc. In this guidebook, we use the Fortran compiler approach.

1. Untar the source file and run `./configure`. For the untar directory is just the installation directory, it is suggested that you copy the source file into the directory `/home/limh/Programs/` before you untar it.
   ```
   $ cp /home/limh/Downloads/Healpix3.11_2013Apr24.tar.gz /home/limh/Programs/
   $ cd /home/limh/Programs
   $ tar -zvxf Healpix_3.11_2013Apr24.tar.gz
   $ ./configure
   ```

   After doing this, you will see a menu with several options. Choose the Fortran compiling options and then follow the self-explanatory guidelines it gives. Do not edit the default compiling options and settings for the compilers if you don’t know what it means. You will be asked to give the name of your Fortran compiler (just type in `ifort`) and the installation path of cfitsio (i.e. `/home/limh/Programs/cfitsio`). When it goes back to the starting menu, type in `'0'` and then press Enter to exit.

2. Run `make` to build the facilities.
   ```
   $ make
   $ make test
   ```
   Seeing a successful message means you have successfully installed HEALPix.

   ```
   process_mask> normal completion
   Healpix F90 tests done
   success rate: 10/10
   ```

E. Building WMAP Likelihood Data

1. Go to [http://lambda.gsfc.nasa.gov/product/map/dr5/likelihood_get.cfm](http://lambda.gsfc.nasa.gov/product/map/dr5/likelihood_get.cfm) to download the source file `wmap_likelihood_full_v5.tar.gz`.

2. Copy the file to the working directory (for me, this is `/home/limh/workspace`). Untar the source file.
   ```
   $ cp /home/limh/Downloads/wmap_likelihood_full_v5.tar.gz /home/limh/workspace
   $ tar -zvxf wmap_likelihood_full_v5.tar.gz
   ```

3. Edit the Makefile. Add the installation path of cfitsio and MKL library of the intel Fortran compiler (the modifications are shown in **boldface**).
   ```
   $ cd wmap_likelihood_full_v5
   $ vi Makefile
   ```
   ```
   CFITSIO=/home/limh/Programs/cfitsio
   ```
   ```
   # Linux/Intel compiler and MKL libraries
   MKLPATH = /home/limh/Programs/intel/composer_xe_2013_sp1.3.174/mkl/lib/intel64
   ```
F90 = ifort
FFLAGS = -02 -fpic $(WMAPFLAGS)
INCS = -I. -I$(CFITSIO)/include
LIBS = -L. -L$(MKLPATH) -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core -liomp5 -lmkl_mc3
          -lmkl_def -lmkl_lapack95_lp64 -L$(CFITSIO)/lib -lcfitsio...

4. Open the WMAP_9yr_options.f90 file. Modify the first line to give the path of the data directory of wmap likelihood full v5 (the modifications are shown in boldface).

   $ vim WMAP_9yr_options.f90

   ... Character(Len=128) :: WMAP_data_dir = '/home/limh/workspace/wmap_likelihood_v5/data/' ...

5. Run make all to build wmap likelihood full v5.

   $ make all

F. Building Planck Data

If you want to use the Planck data in your study, then you have to build it as the WMAP likelihood data. The procedure is somewhat different [6].

1. Go to http://cosmologist.info/cosmomc/readme_planck.html. Use the hyperlink it provides to download the source file plc-1.0.tar.gz.

2. Copy the file to the working directory (for me, this is /home/limh/workspace/). Untar the source file.

   $ cp /home/limh/Downloads/plc-1.0.tar.gz /home/limh/workspace
   $ tar -xzvf plc-1.0.tar.gz

3. Go to the directory and edit the Makefile to give the library path of cfitsio and that of the Intel@Fortran compiler (the modifications are shown in boldface).

   $ cd plc-1.0
   $ vi Makefile

   ... CFITSIOPATH = /home/limh/Programs/cfitsio
   ... # on a linux machine, ifort 11.1
   IFORTLIBPATH = /home/limh/Programs/intel/compiler/intel64
   IFORTRUNTIME = -L$(IFORTLIBPATH) -lintlc -limf -lsvml -liomp5 -lifport -lifcoremt -lpthread
   ...

   Here you can either edit the MKLROOT and LAPACKLIBPATHMKL to give the installation path of the MKL library (you can run echo $MKLROOT to find your own installation path), e.g.

   ... MKLROOT = /home/limh/Programs/intel/compiler/intel64
   LAPACKLIBPATHMKL = -L$MKLROOT/lib/intel64
   ...

   or just leave it empty to be set during configure using the options –lapack_mkl=$MKLROOT.

4. Configure and make. See the instructions on the webpage http://cosmologist.info/cosmomc/readme_planck.html. If you have already set the installation path of the MKL library (i.e. edited the MKLROOT and LAPACK-LIBPATHMKL variables in the Makefile), then you should omit the option --lapack_mkl=$MKLROOT in the following commands. Otherwise, you should just run the following commands:

   $ cd plc-1.0
   $ ./waf configure --lapack_mkl=$MKLROOT --lapack_mkl_version=10.3 --install_all_deps
   $ ./waf install

5. Add the following lines into the .bashrc file in the home directly (for me, this is /home/limh).

   $ vi /home/limh/.bashrc

   ... export PLANCKLIKE=cliklike
   export CLIKPATH=/home/limh/workspace/plc-1.0
   export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$CLIKPATH/lib

   Save and quit. Then run source /home/limh/.bashrc to implement the bash settings.
6. Go the cosmomc root directory (for me, this is `/home/limh/workspace/cosmomc`) and make a static symbolic link to the Planck data.

$ cd /home/limh/workspace/cosmomc
$ ln -s /home/limh/workspace/plc-1.0 ./data/clik

G. Compiling CosmoMC

Having all the prerequisites installed, now we can set out to compile and run CosmoMC. Note that the compile of CosmoMC is carried out in the `cosmomc/source` directory.

1. Go to http://cosmologist.info/cosmomc/readme.html. Use the hyperlink it provides to download the source file `cosmomc.tar.gz`.

2. Untar the source file `cosmomc.tar.gz`.

$ cp /home/limh/Downloads/cosmomc.tar.gz /home/limh/workspace
$ tar -xzvf cosmomc.tar.gz

3. Edit the `Makefile` in the directory `cosmomc/source/` to give the installation path of cfitsio (the modifications are shown in **boldface**).

   $ cd cosmomc/source
   $ vi Makefile

   ```
   WMAP = /home/limh/workspace/wmap
   cfitsio = /home/limh/Programs/cfitsio
   ```

   Here remember not to edit the `PLANCKLIKE` environment variable content even if one wants to use the Planck data in CosmoMC. Because we have already set this in the `.bashrc` file when we build the Planck data. We don’t have to do it again in the Makefile of CosmoMC.

   ...  
   ifeq ($(COSMOHOST), darwin)
   WMAP = /home/limh/workspace/wmap
   cfitsio = /home/limh/Programs/cfitsio
   endif

4. Edit the `Makefile` in the directory `cosmomc/camb/` to give the installation path of cfitsio and Healpix (the modifications are shown in **boldface**).

   $ cd /home/limh/workspace/cosmomc/camb
   $ vi Makefile

   ```
   FITSDIR = /home/limh/Programs/cfitsio
   FITSLIB = /home/limh/Programs/cfitsio/lib
   HEALPIXDIR = /home/limh/workspace/Healpix_3.11
   ```

5. Run `make` and `make getdist`.

   $ make
   $ make getdist

   After running `make getdist`, you will find that a file named `getdist` generated in the cosmomc root directory. Then you can go to the cosmomc root directory to run CosmoMC.

   If you get error message like `libimf.so: warning: feupdateenv is not implemented and will always fail`, just add `-limf` (or `-limf -lm`) to the `FFLAGS` (options of the compiler) in the `Makefile` in the directory `/home/limh/workspace/cosmomc/source`. It tells the compiler to link not only the math libraries of the Intel compilers but also those of the system [5]. The Makefile would look like

   ```
   F90C = ifort
   FFLAGS = -openmp -fast -w -fpp2 -limf
   ```
II. RUNNING COSMOMC AND GENERATING PLOTS

A. On a Desktop

Every time you modify the code, it is recommended that you first ‘make’ the CosmoMC on your own desktop to make sure there is no errors or warnings during the compile. You can use the test.ini or params_generic.ini provided in the root directory of cosmomc to do this. A detailed description of the files and folders in the root directory of CosmoMC is given in the readme.html file in its root directory, which is also available on the website http://cosmologist.info/cosmomc/readme.html.

1. Run and test CosmoMC. You can use ../cosmomc test.ini or mpirun -np 2 . ./cosmomc params_generic.ini to do this.
   $ cd /home/limh/workspace/cosmomc
   $ mpirun -np 2 ./cosmomc params_generic.ini
   This command will generate data file in the /cosmomc/chains directory. For a successful convergent run, you can see the time it takes from the feedback message in the Terminal, e.g.

   Chain 2 MPI Communicating
   Chain 1 MPI Communicating
   Current convergence R-1 = 5.4434482E-03 chain steps = 437
   Requested convergence R achieved
   Total time: 0 ( 0.00011 hours )
   Then one can run mpirun -np 2 ./getdist distgeneric.ini to generate the plot data. Before doing so, one has to manually create a folder named plot_data in the root directory of CosmoMC (for me, this is /home/limh/workspace/cosmomc).

2. Create the plot_data folder and generate the plot data.
   $ cd /home/limh/workspace/cosmomc
   $ mkdir plot_data
   $ mpirun -np 2 ./getdist distgeneric.ini

3. Use Python to generate the plots. Before doing this, one has to copy all the files in the cosmomc/python/ directory (most essential the GetDistPlot.py) to the root directory of CosmoMC (for me, it is /home/limh/workspace/cosmomc).
   $ cp /home/limh/workspace/cosmomc/python/*.* /home/limh/workspace/cosmomc

4. Then you can go to the Ubuntu Software Center to download and install the IDLE(using Python-2.7) (an integrated development environment for python using Python-2.7).
   (1) After successfully installing IDLE(using Python-2.7), click the icon to start it. It will start a new window titled ‘Python 2.7.6 Shell’.
   (2) Click ‘File → Open’, go to the directory /home/limh/workspace/cosmomc and choose test.py (or test_tri.py) to open. Then another window will pop out, displaying the content of the ‘test.py’ file (or ‘test_tri.py’ file).
   (3) Then press F5 on the keyboard to run the script. If everything works fine, there would be a pdf file named test.pdf (or test_tri.pdf) generated in the directory /home/limh/workspace/cosmomc. That is the parameter plot one expects from the CosmoMC.

B. On a Cluster

A full implementation of CosmoMC needs a cluster environment. To have it run on a cluster, one should first successfully make it (see Section II, A. Compiling CosmoMC) on his own desktop. Then one has to write a job-submit script in the root directory of CosmoMC and have it run in the Terminal of the cluster. A job-submit script is just a text file written in the bash language telling the cluster how to run the program. It specifies the root directory of CosmoMC, the nodes and cores on which you want to run CosmoMC, and the name and path of the output files in which you want the feedbacks and error messages (if there are any) to be saved, etc. Samples of a PBS(Protable Batch System) job-submit script are easy to obtain on the Internet.

Here we give our job-submit script sample below. It is written as neatly as possible for the beginners. One can copy the file and edit it as appropriate for your own machine. It is named limhsub.sh and placed in the directory /ihepbatch/mbhd01/user/liyangrong/liminghua/limh/cosmomc/ on the cluster.

 adamkroft@gmail.com

*******************************************************************************
#!/bin/bash
#PBS -N limhsub.sh
#PBS -o /ihepbatch/mbhd01/user/liyangrong/liminghua/limh/limhsub.out
#PBS -e /ihepbatch/mbhd01/user/liyangrong/liminghua/limh/limhsub.err
#PBS -l nodes=2:ppn=8

DIR_HERE=/ihepbatch/mbhd01/user/liyangrong/liminghua/limh/cosmomc
DIR_MPI=/ihepbatch/mbhd01/user/liyanrong/liminghua/Programs/openmpi/bin

cat $PBS_NODEFILE > $DIR_HERE/hostfile
NCPU=`wc -l < $PBS_NODEFILE`

source /ihepbatch/mbhd01/user/liyanrong/liminghua/.bashrc
cd $PBS_O_WORKDIR
$DIR_MPI/mpirun -hostfile `$(PBS_NODEFILE)` -np $NCPU $DIR_HERE/cosmomc $DIR_HERE/params_generic.ini

## The following lines are annotations.
## The first line `#!/bin/bash` is not an annotation. It tells the cluster that this script is written in the bash language.
## The second to fifth lines that starts with `#PBS` are not annotations. They are the command lines of the PBS system.
## The fifth line means using 2 nodes to run the CosmoMC. Each node uses 8 cores.
## The seventh and eighth lines respectively gives the path of the working directory of CosmoMC and Open MPI.
## The tenth line uses the bash command `cat` to show the content of the file `$PBS_NODEFILE` and write into a new file named `hostfile` in the root directory of CosmoMC.
## The eleventh line counts the number of available nodes and save it in the variable `$NCPU`.
## The thirteenth line `source ...` is necessary for the cluster to recognize the Intel@Fortran compiler, Open MPI, and the Planck dataset etc.
## The fourteenth line is to go to the working directory `$DIR_HERE`. Thus the cluster can identify the directory paths in the codes that are given with respect to the root directory of CosmoMC.
## The last line tells the cluster to run the `cosmomc` file with its options-file `params_generic.ini`. `-np` and `--hostfile` is the options of Open MPI. Appropriate options should be used for specific cluster environments. For example, an Infiniband- or Ethernet-communicating cluster demands different MPI options. See `http://www.open-mpi.org/faq/?category=openfabrics#ib-btl` for more information.
## If you have any troubles in doing this, you can:
## (1) Run `mpirun --help` in the Terminal for a brief introduction of the options;
## (2) Go to the FAQ of Open MPI mailing lists `http://www.open-mpi.org/faq/?category=openfabrics#ib-btl` for more information (we find this very helpful);
## (3) Contact the system administrator to get more support.

To submit a job-submit script, one can use the command `qsub`, following the name of the script file. For more information about job submission, just `google` the Torque or PBS system, or consult with your system administrator for more support.

### C. FAQs about Running

1. (On a cluster) If you have limited registered memory error messages in your `.err` file like:
   `libibverbs: Warning: RLIMIT_MEMLOCK is 32768 bytes.
   This will severely limit memory registrations.
   ...
   `and the `.out` file like
   The OpenFabrics (openib) BTL failed to initialize while trying to allocate some locked memory. This typically can indicate that the memlock limits are set too low. For most HPC installations, the memlock limits should be set to "unlimited". The failure occured here:
Local host: mbh023
OMPI source: btl_openib.c:872
Function: ompi_free_list_init_ex_new()
Device: mlx4_0
Memlock limit: 32768
... you may need to consult with your system administrator to get this problem fixed [7].

2. (On a desktop or cluster) If you get error message like:

libimf.so: warning: feupdateenv is not implemented and will always fail
... just add `-limf` (or `-limf -lm`) to the FFLAGS (options of the compiler) in the Makefile in the source folder in the root directory of CosmoMC (for me, this is /home/limh/workspace/cosmomc/source). It tells the compiler to link not only the math libraries of the Intel compilers but also those of the system [5]. The Makefile would look like

... F90C = ifort
FFLAGS = -openmp -fast -w -fpp2 -limf
...

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[1] http://www.cuhk.edu.hk/itsc/compenv/research-computing/orion/cosmomc.html.
[2] http://159.226.251.229/videoplayer/COSMOMC.pdf?ich_u_r_i=944ae037f9549b9e96ee29f6b562b8c1&ich_s_u_r_i=0&ich_e_n_d=0&ich_k_e_y=1445078930750263292451&ich_t_y_p_e=1&ich_d_i_s_k_i_d=6&ich_u_n_i_t=1.
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