

Introduction to CosmoMC

Part II: Installation and Execution

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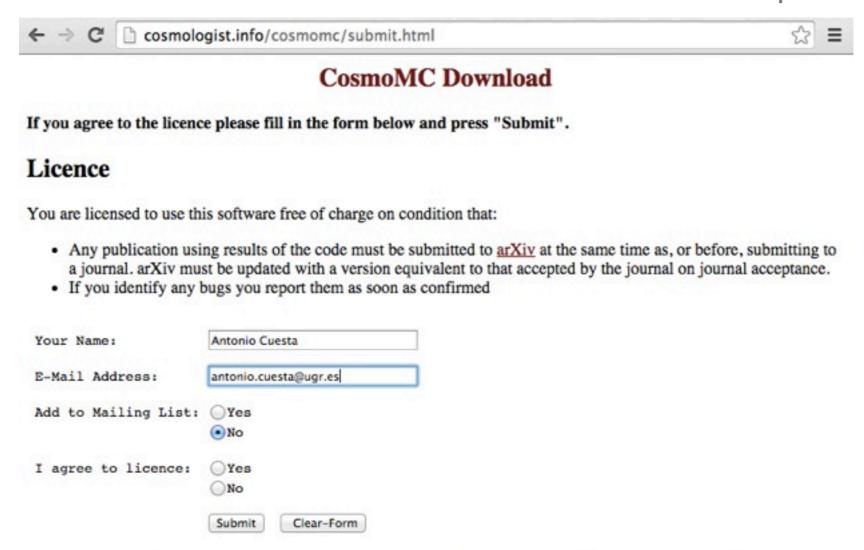
Outline of Part II

- Downloading and Installing CosmoMC
- Customizing Params.ini: datasets and model parameters
- Running the code: the script runMPI.py
- Testing for chain convergence
- Finding the maximum likelihood values
- Post-processing: Importance sampling

Downloading CosmoMC

Go to http://cosmologist.info/cosmomc/submit.html

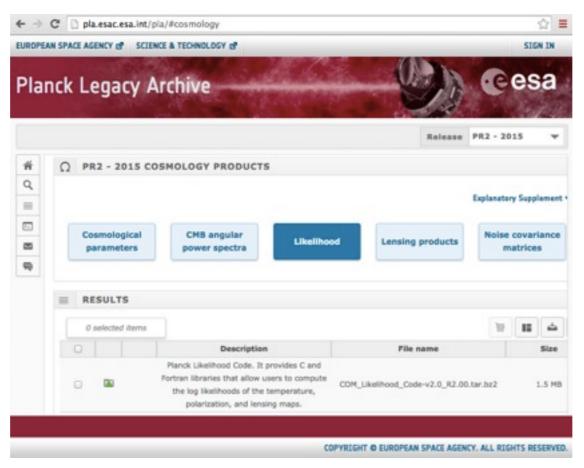
You will receive an email with links to download current and previous versions



You are encouraged to add yourself to the mailing list - you will then be informed about any bugs, and will also get news of new versions.

Installing Planck likelihood

• This is technically NOT part of CosmoMC, but **you will need it** every time, so when you install CosmoMC, you want to install this all together.



You have to download at least two files (300MB): the likelihood code COM_Likelihood_Code-v2.0_R2.00.tar.bz2 and the data files COM_Likelihood_Data-baseline_R2.00.tar.gz (that contains hi_l, low_l, lensing)

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"Introduction to CosmoMC" Part II

Installing Planck likelihood

- Installation is done by running these two commands:
 - ./waf configure --lapack_mkl=\${MKLROOT} --install_all_deps
 - ./waf install
- We will not need to do this, since it is already installed in *ftaecluster*, but we
 do need to set up the environment so that CosmoMC can find the files:
 source ./bin/clik_profile.sh
- You just need to create a symbolic link to your Planck2015 likelihood directory (plc_2.0) to a folder named 'clik' inside cosmomc/data/
 ln -s /path/to/planck/2015/plc 2.0 /path/to/cosmomc/data/clik
- NOW you can compile!

Installing CosmoMC

LAPACKL =

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- Unfortunately current version of CosmoMC requires a commercial compiler (Intel Fortran Compiler, part of Intel Parallel Studio XE), a.k.a. "ifort"
- The (free) GNU Fortran compiler "**gfortran**" could in principle be used, but current released versions (including v5.3.0) do not work, but dev-v6.0 does. Performance is not expected to match ifort, but at least it is free

```
OUTPUT DIR ?= Release
BUILD ?= MPI
                                                                      Edit this file: source/Makefile
#set BUILD to MPI to force MPI, should be set in ../Makefile
MPIF90C ?= mpif90 -f90=ifort MPI compiler
                                                                                         make
                                                                                  make install
ifortErr = $(shell which ifort >/dev/null; echo $$?)
#these settings for ifort 14 and higher. Earlier versions will not work.
ifeq "$(ifortErr)" "0"
#ifort; Can remove -xHost if your cluster is not uniform, or specify specific processor optimizations -x...
        = ifort Fortran compiler
#use this if mpif90 is trying to use gfortran: MPIF90C = mpif90 -f90=ifort
FFLAGS = -mkl -openmp -03 -no-prec-div -fpp Flags for optimization, openMP parallelization, and link to Intel MKL library
DEBUGFLAGS = -mkl -openmp -g -check all -check noarg_temp_created -traceback -fpp -fpe0
#add -fpe0 to check for floating point errors (think lowLike also throws these harmlessly)
MODOUT = -module $(OUTPUT_DIR)
```

Use the <u>same</u> compiler for Planck and CosmoMC !!

"Introduction to CosmoMC" Part II

Parameter files

- This code has **two** main parameter files:
 - params.ini, the parameter file for CosmoMC,
 which sets up the chains (cosmological model and datasets)
 - distparams.ini, the parameter file for GetDist,
 which sets up the analysis (figures and statistics)
 - There are many other (minor) settings contained in other files. If you have a specific need, it will most likely be contained in those other files!

params.ini : File structure

- This file contains all the settings for your MCMC chains. It can have any name, but we will refer to it as **params.ini**.
- The settings can be (and actually are) nested, i.e. inside params.ini you can INCLUDE or DEFAULT another settings file. This is called **nesting**
- INCLUDE will add the new settings if they are not previously defined
- DEFAULT will override previously defined settings if there is a conflict
- Note that the main file which is nested inside params.ini is **batch2/ common.ini**, where the variable MPI Converge Stop is set.

params.ini: Basic settings

• First, you want to name your chain. Tip: the name should contain information about the **cosmological model**, and about the **datasets** used (e.g. 'OLCDM_Planck2015_BAO')

```
#Folder where files (chains, checkpoints, etc.) are stored
root_dir = chains/
#Root name for files produced
file_root=planck15dr12
```

Second, you want to run a MCMC chain. So make sure that the setting action in params.ini is set to zero (action=0). By default it is set to test likelihoods (action=4). Note that you can also find the best-fitting values of your cosmological parameters given the datasets (action=2) or add a new dataset to existing chains via importance sampling (action=1)

```
#action= 0 runs chains, 1 importance samples, 2 minimizes
#use action=4 just to quickly test likelihoods
action = 0
```

You can also change the **temperature** in your chains, i.e. sample the distribution $P^{1/T}(x)$ rather than P(x). High temperature will explore tails better.

params.ini: Choosing your datasets

• Select the datasets (likelihoods) to be used. Comment out (using '#' symbol) the ones you don't need. Include the ones you want with DEFAULT

All the built-in likelihoods are installed in the *batch2*/ directory
You can define yours too (take *batch2/HST.ini* as a good starting example)

```
#general settings
#Bicep-Keck-Planck, varying cosmological parameters
#DEFAULT(batch2/BKPlanck.ini)
#Planck 2015, default just include native likelihoods (others require clik)
DEFAULT(batch2/plik_dx11dr2_HM_v18_TTTEEE.ini) Planck2015 highL temperature+polarization
                                             Planck2015 lowL temperature+polarization
DEFAULT(batch2/lowTEB.ini)
#DEFAULT(batch2/lowl.ini)
                                             Planck2015 lowL temperature only
#DEFAULT(batch2/lensing.ini)
                                             Planck2015 CMB lensing
#Other Likelihoods
                                             BAO from BOSS+MGS+6dF(+WiggleZ)
#DEFAULT(batch2/BAOnew.ini)
                                             WiggleZ galaxy power spectrum
#DEFAULT(batch2/WiggleZ_MPK.ini)
                                             SDSS galaxy power spectrum
#DEFAULT(batch2/MPK.ini)
                                             CFHTLens weak lensing
#DEFAULT(batch2/WL.ini)
```

Also, SNe from JLA, etc.

for example, for CMB from PLANCK, you typically want to include a low- ℓ likelihood, a high- ℓ likelihood, and (sometimes) a CMB lensing likelihood.

params.ini : Setting your parameters

- In CosmoMC there are **three** types of parameters:
- Cosmological parameters: these are the ones you want to vary, as part of the cosmological model you choose. The default is the 6 ΛCDM base parameters
- Nuisance parameters: these you are forced to vary when you include some particular datasets (e.g. Planck, JLA) because this is the way to marginalize over systematics effects. They are added automatically when you use that data
- **Derived** parameters: these are not varied themselves, but they depend on cosmological parameters ($\Omega_{\rm m}^{0.3}\sigma_8$), so you indirectly obtain constraints on them They are marked with a star (*), see paramnames/derived_.paramnames

They will all included in your chains explicitly, so you can check that everything is OK by looking at your chains or the *paramnames file generated in the directory cosmomc/chains

params.ini : Setting your parameters

 The priors of the 6 LCDM parameters are defined in the file batch2/params_CMB_defaults.ini

Change them here if you need to, or (better) re-define them again in your params.ini, which has higher priority. Follow this syntax:

```
#to vary parameters set param[name] = center, min, max, start width, propose width
#param[mnu] = 0 0 0 0 0
```

- Basically write a fiducial (a guess) starting value, a left and a right bound (hard priors), and two numbers you guess for the uncertainties
- You can of course include additional non-LCDM parameters defined in CAMB A complete list is in the file paramnames/params CMB.paramnames

```
param[omegak] = 0 - 0.1 \ 0.1 \ 0.005 \ 0.005
param[w] = -1 - 3 \ 1 \ 0.05 \ 0.05
param[wa] = 0 - 3 \ 3 \ 0.3 \ 0.3
```

Running the code

- Remember that this is a *PARALLEL* code! Although it can be run in any machine (provided that it meets the compiling requirements), it only makes sense to run it in multi-processor machines (not on your laptop)
- The code has **OpenMP/MPI** parallelization implemented. That basically means that you can run the code in parallel using processors in the same node (OpenMP) or in different nodes (MPI). Or, better, combine both
- The typical workload distribution to get the best of both parallelization schemes: communication between chains uses MPI and each chain uses as many processors as possible = #processors_per_node / #chains_per_node
- In the practice session, we will use 1 node per person, so MPI communication will be INSIDE the same node

The script python/runMPI.py

- OpenMP is controlled by the environment (bash) variable OMP_NUM_THREADS
 MPI is set up with the option -n of mpirun / mpiexec
- In a computing cluster like *ftaecluster*, we typically need to write a **job file** for the torque/moab/slurm scheduler to set up the **resources** the code needs and the **command** to be run

```
#!/bin/bash
#PBS -q batch
                                Queue name
#PBS -l nodes=1:ppn=16
                                Nodes used
#PBS -l walltime=240:00:00
                                time required
#PBS -N lcdmdr12
                                 iob name
#PBS -r n
#PBS -W group list=icc
                                standard and
#PBS -o out/lcdmdr12.out
                                error outputs
#PBS -e out/lcdmdr12.err
cd /home/acuesta/cosmomc2015jul
export OMP_NUM_THREADS=2
source planck2015.sh; time /opt/mpi/bullxmpi/1.0.2/bin/mpirun -n 8 ./cosmomc lcdmdr12.ini > ./scripts/lcdmdr12.log 2>&1 &
wait
```

This is what you'd always need to write in order to run a code in *ftaecluster*.
 But fortunately, CosmoMC simplifies this task by using the script **runMPI.py**

The script python/runMPI.py

• The script **python/runMPI.py** uses an alternative way to submit runs to the computing cluster by just using a 1-line command, e.g.:

```
python python/runMPI.py --nodes 1 --chainsPerNode 8 --coresPerNode 16 --mem_per_node 40000
--walltime 480:00:00 --job_template job_script_hipatia --program ./cosmomc --queue batch ow0wacdmbaosn.ini
```

- This basically gives the same information as before, but you don't need to write a file to submit a run -- you just write a **command**
- However, this requires that the cluster configuration is correctly specified in the job_script file, which you have to customize (only once!) to your cluster
- In the case of ftaecluster, you can use the file job_script_ftaecluster provided. Remember to change this if the cluster configuration changes!

How to minimize runtime

- This is usually given by your own experience, but there are general guidelines:
- OpenMP speeds up a chain by computing in parallel each call to CAMB ('slow' steps, when the transfer function needs to be recomputed).

- MPI is used to communicate between chains. This happens rarely, when the code decides to update the covariance matrix of your parameters from the information in the already running chains, adapting the step size
- Remember also to include in your parameter file a propose_matrix as close as possible to your model+dataset combination

How to minimize runtime

- I would recommend this typical set-up:
- at least 8 chains per code execution (therefore you will start with 8 different initial conditions to sample your parameter space). If the node has 16 processors (ftae, nodes 1-7), that means OMP_NUM_THREADS=2. If the node has 32 processors (ftae, nodes 8-9) that means OMP_NUM_THREADS=4
- If there are many nodes available, in principle you can run 1 chain per node
 #PBS -1 nodes=8:ppn=16
- In practice, you want to run several cosmological models or several dataset combinations at the same time, so all chains in the same node
 #PBS -1 nodes=1:ppn=16

MCMC Chain files

- A chain file is just a text file, you can open it with any editor or use it through any python script (or the way that is most convenient for you)
- Each row is a MCMC step. Each column is each one of the parameters in this order: cosmological, nuisance, and derived. The first two columns are the multiplicity (or number of steps spent in that point) and the -log(likelihood), or "loglike", which is just 0.5 times the total χ^2 value.

mult & loglike LCDM parameters

721827E+00 0.2234986E+00 0.1081429E+02 0.1822413E+01 0.4143067E+02 0.1381347E+05 0.1333238E+02

.1240745E+00 0.1117157E+00 0.3490495E+00 0.5606420E+00 0.1334311E+00 0.1757612E+00 0.3807932E+00 0.2035620E+00 0.6760326E+00 0.1314555E+01 0.9986082E+00 0.9941414E+00 0.6677979E+ 02 0.6774565E+00 0.3225435E+00 0.1438396E+00 0.6451439E-03 0.9605576E-01 0.8370669E+00 0.4753947E+00 0.6308226E+00 0.1024325E+01 0.2523461E+01 0.1168060E+02 0.2214488E+01 0.182 5188E+01 0.1206639E+04 0.5520434E+04 0.2454898E+04 0.7891323E+03 0.2233522E+03 0.9647925E+00 0.2453066E+00 0.2466328E+00 0.2627639E+01 0.1382655E+02 0.1040935E+01 0.1386405E+02 0.1059551E+04 0.1470385E+03 0.1407766E+00 0.1609642E+00 0.3421912E+04 0.1044400E-01 0.8091325E+00 0.4473433E+00 0.1147113E+00 0.7956448E+02 0.1001239 E+84 0.3507600E+00 0.7098143E-01 0.9268106E+02 0.1398548E+04 0.6788087E+00 0.4943056E+00 0.7053466E+00 0.4894761E+00 0.6200091E+00 0.3953857E+04 0.1049665E+05 200932E+00 0.5372448E+00 0.7533748E+01 0.7409717E+00 0.2005705E+02 0.1445050E+05 0.9032058E+01 0.2000000E+01 0.7432273E+04 0.2205772E-01 0.1223525E+00 0.1040409E+01 0.9243788E-01 0.3091427E+01 88E-01 0.2326024E+00 0.3234647E+03 0.4471673E+02 0.1465753E+02 0.8721921E+02 0.5519028E+01 0.4040853E+01 0.8603040E+01 0.2843156E+02 0.8216804E+02 0.6988734E-01 0.8529992E-01 0 .1473713E+00 0.1212628E+00 0.4138422E+00 0.5325758E+00 0.2066227E+00 0.204037E+00 0.3101160E+00 0.2384299E+00 0.6598682E+00 0.1248762E+01 0.9968187E+00 0.9981910E+00 0.6611572E+ 0.0681633E+00 0.3318367E+00 0.1450554E+00 0.6451439E-03 0.9590442E-01 0.8370717E+00 0.4821974E+00 0.6353218E+00 0.1029462E+01 0.2543836E+01 0.1138763E+02 0.2200845E+01 0.182 9359E+01 0.1218436E+04 0.5524315E+04 0.2451456E+04 0.7855802E+03 0.2219278E+03 0.9585111E+00 0.2452473E+00 0.245732E+00 0.2650759E+01 0.1385349E+02 0.1090526E+04 0.1440652E+03 0.1040627E+01 0.1384408E+02 0.1059361E+04 0.1468229E+03 0.1409091E+00 0.1610448E+00 0.3450975E+04 0.1053267E-01 0.8034780E+00 0.4444658E+00 0.1137244E+00 0.7910790E+02 0.1009162 E+04 0.3515068E+00 0.7049756E-01 0.9239276E+02 0.1407670E+04 0.6811109E+00 0.4986407E+00 0.7037144E+00 0.4916913E+00 0.6178100E+00 0.3612763E+04 0.1049756E+05 0.6964181E+03 0.4 869998E+00 0.1972903E+00 0.1102911E+02 0.1891800E+01 0.4420137E+02 0.1411032E+05 0.1360520E+02 0.4000000E+01 0.7284871E+04 0.2198426E-01 0.1221917E+00 0.1040366E+01 0.1098112E+00 0.3125897E+01 0.9607862E+00 0.1000165E+01 0.1525372E+00 0.3207994E+01 0.8596888E+02 0.10553 51E+00 0.3467409E+01 0.2893997E+03 0.4493034E+02 0.2553329E+02 0.7202911E+02 0.6357391E+01 0.1250935E+02 0.8857744E+01 0.2133231E+02 0.6452248E+02 0.6871896E-01 0.7897106E-01 0 .1537515E+00 0.1198039E+00 0.4199892E+00 0.5379834E+00 0.1532049E+00 0.1571962E+00 0.4808829E+00 0.2579597E+00 0.7759683E+00 0.1462243E+01 0.9989428E+00 0.9984782E+00 0.6609619E+ 0.148211E+00 0.6451439E-03 0.9572121E-01 0.8520634E+00 0.4905817E+00 0.6465344E+00 0.1048054E+01 0.2582354E+01 0.1288300E+02 0.278031E+01 0.182 8854E+01 0.1221446E+04 0.5509919E+04 0.2451231E+04 0.7856986E+03 0.2223143E+03 0.9607862E+00 0.2452129E+00 0.2465387E+00 0.2665088E+01 0.1386161E+02 0.1090606E+04 0.1441621E+03 0.1040593E+01 0.1385383E+02 0.1059208E+04 0.1469439E+03 0.1407185E+00 0.1611494E+00 0.3445374E+04 0.1051558E-01 0.8042171E+00 0.4449052E+00 0.1137728E+00 0.7907232E+02 0.1009537 E+04 0.3514796E+00 0.7052297E-01 0.9234238E+02 0.1408265E+04 0.6810272E+00 0.5074146E+00 0.7163785E+00 0.5004196E+00 0.6289566E+00 0.3312784E+04 0.1050069E+05 0.7015079E+03 0.4

1MCMC step

MCMC Chain files

• The column ordering can be found in the file chains/root.paramnames

```
omegabh2
                \Omega_b h^2
omegach2
                \Omega_c h^2
       100\theta_{MC}
        {\rm{ln}}(10^{10} A_s)
logA
calPlanck
                y_{\rm cal}
alpha_JLA
                \alpha_{JLA}
beta_JLA
                \beta_{JLA}
acib217 A^{CIB}_{217}
       \xi^{tSZ-CIB}
asz143 A^{tSZ}_{143}
aps100 A^{PS}_{100}
aps143 A^{PS}_{143}
                A^{PS}_{143\times217}
aps217 A^{PS}_{217}
       A^{kSZ}
kgal100 A^{{\rm dust}TT}_{100}
kgal143 A^{{\rm dust}TT}_{143}
kgal143217
                A^{{\rm dust}TT}_{143\times217}
kgal217 A^{{\rm dust}TT}_{217}
                A^{{\rm dust}EE}_{100}
galfEE100
galfEE100143
                A^{{\rm dust}EE}_{100\times143}
galfEE100217
                A^{{\rm dust}EE}_{100\times217}
                A^{{\rm dust}EE}_{143}
galfEE143
galfEE143217
                A^{{\rm dust}EE}_{143\times217}
                A^{{\rm dust}EE}_{217}
galfEE217
                A^{{\rm dust}TE}_{100}
galfTE100
                A^{{\rm dust}TE}_{100\times143}
galfTE100143
                A^{{\rm dust}TE}_{100\times217}
galfTE100217
                A^{{\rm dust}TE}_{143}
galfTE143217
                A^{{\rm dust}TE}_{143\times217}
                A^{{\rm dust}TE}_{217}
galfTE217
        c_{100}
cal2
        c_{217}
       H_0
omegal* \Omega_\Lambda
omegam* \Omega m
```

This file has two columns: the internal name of the parameter and a LaTeX script so that the plots display their name properly (edit this file to your convenience)

Convergence: Gelman-Rubin criterion

- The *R-1* estimator (Gelman and Rubin 1992) is defined roughly as "the variance of the chain means divided by the mean of the variances". A set of chains is declared **converged** when this estimator is **small** enough (typically 0.01)
- This is computed for **EACH** parameter. Typically the value you quote to assess the convergence of your chain is the worst (**largest**) value over all parameters
- Each chain will have a (slightly) different mean but the dispersion between chains is small compared to the mean error bar when converged

$$\hat{R} = \sqrt{\frac{\hat{\mathrm{Var}}(\theta)}{W}}$$

$$\hat{\text{Var}}(\theta) = (1 - \frac{1}{n})W + \frac{1}{n}B$$

where W is the "within chain" variance and B is the "between chains" variance of the means

if the chain is more or less converged R will be a little bit over 1.0 convergence is measured by the value of R-1

How to check progress of your chains

- In the directory **cosmomc/scripts** there will be a file constantly updated named **root.log**, where *root* is the name you gave to your chains in *params.ini*
- Open that file and search the word "convergence". You will find several instances like this:

Current convergence R-1 = 0.1990366 chain steps = 1370

- The last occurrence gives you an idea of the current chain convergence and how far you are from the target value MPI_Converge_Stop (default 0.01)
- Another (better) way to obtain R-1 is to run GetDist (session 3)

Find maximum likelihood (action=2)

- MCMC is **not optimized** to find a maximum, but to sample parameter spaces (Metropolis-Hastings is NOT a gradient method like downhill simplex etc). The bestfit value given at the **likestats** file (see session 3) will be **approximate**
- This uses Powell 2009 BOBYQA minimization. The code starts at the "center" parameter values in the .ini file, and requires that the likelihood does not return NaN in the region between those values
- It stops at a given value given by minimize_loglike_tolerance given that the true minimum is within max_like_radius (in units of the parameter error). All these settings are found at **batch2/common.ini**
- The output is then given in root.minimum

Importance sampling (action=1)

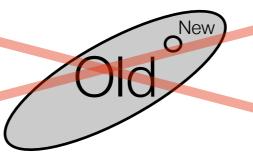
- Sometimes you want to explore the effect of an additional dataset on your chains that you already run with your favorite model+dataset combination.
 (For example: you want to see the effect of a recent measurement of H0 on your chains that you ran for CMB+BAO+SN in the ΛCDM model)
- In principle you would need to run a new chain, which is slow.
 But this can be done much faster by re-weighting each step of your chains (the re-weighting factor depends on the new data), only if the following two requirements are met:

Importance sampling (action=1)

• 1) The new measurement is **consistent** with the constraints from the chain. That means, if your new data falls away from the allowed parameter space, your resulting constraints will not be reliable since you did not have points to reweight to begin with!

• 2) The new data is **not too constraining**. If the error bar of the new data is small compared with the allowed region in your chains, most points will be reweighted to zero except for a small subset, and your constraints will be noisy.

The opposite case (new data has a very large error bar) can be applied though! but all the points will be reweighted by the same value, so that will have no effect whatsoever



Importance sampling (action=1)

- If you have *.data files this is fast and easy (~10 min). In your parameter file set action=1 and redo_add=T and include the likelihoods you want to add. Or if you set redo_add=F just include all the likelihoods you want included (if a likelihood was included in the old chains, it will not be included twice)
- To create *.data files set the variable indep_sample to some number where the steps are not correlated (GetDist will tell us this), also because *.data files will contain Cℓ and P(k,z) and occupy disk space. Set it to more than 10.
- If you don't have .data files you can still use redo_from_text to do the sampling from the chain files (*.txt), but this is slow and does not work well

Background parametrization

- When no CMB likelihoods are going to be used, then a good choice is the parametrization=background option. This is useful to constrain only parameters **not** related to perturbations (e.g. not $\{A_s \ n_s \ \tau\}$ but $\{H_0 \ \Omega_m \ \Omega_k \ \Omega_v \ w\}$)
- parametrization=background is included in batch2/common.ini.
 Also useful would be to create a file similar to params_CMB_defaults.ini in which the perturbation parameters {A_s n_s τ} are set to constant values, and force bbn_consistency to F
- The current version of the file **likelihood_paramsCMB.f90** sets $\Omega_c h^2 = 0$, and $\tau = 0$, and $\Omega_b = \Omega_m \Omega_v$. This is obviously a bug, so it needs to be replaced and **recompiled**. Also note that Ω_b needs to be constrained by some dataset, or just fixed to some standard value.