FROM BEYONDPLANCK TO COSMOGLOBE:
OPEN SCIENCE, REPRODUCIBILITY, AND DATA LONGEVITY

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ABSTRACT

The BeyondPlanck and CosmoGlobe collaborations have implemented the first integrated Bayesian end-to-end analysis pipeline for CMB experiments. The primary long-term motivation for this work is to develop a common analysis platform that supports efficient global joint analysis of complementary radio, microwave, and sub-millimeter experiments. A strict prerequisite for this to succeed is broad participation from the CMB community, and therefore the program are reproducibility and Open Science. In this paper, we discuss our efforts toward this aim. We also discuss measures toward facilitating easy code and data distribution, community-based code documentation, user-friendly compilation procedures, etc. This work represents the first publicly released end-to-end CMB analysis pipeline that includes raw data, source code, parameter files, and documentation. We argue that such a complete pipeline release should be a requirement for all major future and publicly-funded CMB experiments, noting that a full public release significantly increases data longevity by ensuring that the data quality can be improved whenever better processing technologies, complementary datasets, or more computing power become available, and thereby also taxpayers’ value for money; providing only raw data and final products is not sufficient to guarantee full reproducibility in the future.

1. INTRODUCTION

Reproducibility and replicability are two of the defining features of modern science. Within the field of CMB cosmology, this has most typically been realized in the form of competition between different experiments, each trying to measure the same sky signal but with different instrumentation and analysis techniques.1 This approach has been tremendously successful and has led to a cosmological concordance ΛCDM model that is able to statistically describe nearly all currently available cosmological observables with only six free parameters (Planck Collaboration VI 2020).

The next major milestone for the CMB field is the potential detection of primordial gravitational waves and large-scale B-mode polarization (e.g., Kamionkowski & Kovetz 2016). If successful, this measurement will have far-reaching implications for our understanding of physics at ultra-high energy scales and the creation of the universe. However, this is also an extremely technologically challenging measurement because of the very faint expected signal amplitude. According to current theories and limits, it is anticipated to account for no more than a few tens of nanokelvin fluctuations on large angular scales, which is to be compared with the amplitude of the CMB solar dipole of $3.4\,\text{mK}$ (Fixsen 2009), and with polarized astrophysical foreground contamination of tens of microkelvins (e.g., Planck Collaboration IV 2018). A robust detection will therefore require a relative instrumental calibration better than $O(10^{-5})$ and foreground suppression better than two orders of magnitude (e.g., Gjerløw et al. 2023; Svalheim et al. 2023).

As discussed by BeyondPlanck (2023), this challenge imposes substantial requirements in terms of analysis and modeling techniques. Most notably, because of the intimate relationship between instrument calibration and astrophysical component separation, it is very likely that the associated parameters must be explored jointly, and it is also quite possible that data from different sources and experiments must be analyzed jointly to break internal degeneracies that exist within each experiment separately. As a concrete example, despite having almost one hundred times as many detectors

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1 See, e.g., https://en.wikipedia.org/wiki/List_of_cosmic микроволн_эксперименты for a list of previous, current, and future CMB experiments.
as Planck (Planck Collaboration I 2020) and more than one order of magnitude higher map-level large-scale polarization sensitivity, LiteBIRD’s (LiteBIRD Collaboration et al. 2022) intensity sensitivity will not match Planck’s, and the ultimate LiteBIRD data analysis will therefore undoubtedly directly involve Planck measurements.

There is every reason to expect this to hold true for virtually all current and planned CMB experiments. The data from these experiments will benefit significantly from, if not on a joint analysis with other datasets within iterative pipelines. Such an approach will maximize the amount of secondary science extracted from the datasets and allow them to achieve their primary science goals. Without exception, every single CMB experiment fielded to date has had parameters to which it was not sufficiently sensitive on its own, whether due to its observation strategy, detector design, or frequency coverage. It has typically required massive efforts to devise algorithmic priors or tricks to self-consistently mitigate these “blind spots” or “poorly measured modes”. However, the optimal solution to solving such problems is, of course, by combining datasets with different blind spots, such that one experiment can break the degeneracies observed by another. One concrete example of this is the current BeyondPlanck analysis, which re-analyzes the Planck LFI observations within a Bayesian end-to-end framework, and uses WMAP data to break important degeneracies between large-scale CMB polarization modes and the LFI gain (BeyondPlanck 2023; Gjerløw et al. 2023). Conversely, the ongoing WMAP re-analysis by Watts et al. (2023) will hopefully be able to constrain WMAP’s transmission imbalance parameters using information from Planck, and, if successful, this will improve the data quality of both experiments. Similarly, once LiteBIRD data become available, both WMAP and Planck should be re-analyzed from scratch, exploiting the LiteBIRD’s state-of-the-art large-scale polarization information to further improve the gain models of both experiments. In general, we therefore argue that for this type of joint analysis to be possible, it is critically important for all involved experiments to provide both raw data and a fully operational data analysis pipeline that can be re-run by external scientists.

A main goal of Cosmol oglobe is to establish a common platform for this type of joint analysis that can process low-level uncalibrated CMB time-ordered data (TOD) from different sources directly into high-level astrophysical component maps and cosmological parameters. The first application of this work is a full re-analysis of the Planck LFI observations (BeyondPlanck 2023, and references therein), while extensions to WMAP (Watts et al. 2023), LiteBIRD (LiteBIRD Collaboration et al. 2022), SPIDER (SPIDER Collaboration et al. 2021), COBE-DIRBE (Hauser et al. 1998) and others are on-going. However, for this work to be successful as a community-wide enterprise, it is necessary for all researchers to be able to reproduce the existing work, and integrate their own datasets into the analysis. As such, Open Science and reproducibility plays a critical role in this program.

In this paper, we summarize our efforts on reproducibility within the context of BeyondPlanck and Cosmol oglobe. Its main goals are two-fold. First, it outlines the Open Source implementation of these projects and represents a valuable starting point for other experiments aiming to contribute to and build on this framework. Second, we hope that this paper may serve as a reference for any future astrophysics and cosmology collaboration that wants to perform its work in an Open Source setting; the issues and tasks that need to be addressed in the context of BeyondPlanck and Cosmol oglobe are very likely to be similar for any other project of a similar type. As such, a significant fraction of this paper is spent on surveys of tools and topics that were explored during the initial phases of the project but not ultimately chosen simply because this material may be helpful for other collaborations.

It is important to emphasize that Open Source initiatives are common in astronomy & astrophysical settings. For example, the Astropy Project — the community-driven initiative with the primary goal of developing the core astronomy package in Python. Others include but are not limited to OpenAstronomy, Cosmo-Statistics, Deep Skies, and Dark Machines. Furthermore, a number of astrophysical codes and libraries were developed throughout the years, among which the particularly important for CMB are CAMB, Lewis et al. 2000; Lewis 2004; Challinor & Lewis 2001, CosmoMC, Lewis & Bridle 2002; Lewis 2013, TOAST, FGBuster, Zonca et al. 2019, and many others, most of which have convenient Python wrappers to ease the usage. In addition, the reproduction of Planck 2018 power spectra was done by Li et al. (2021) using the Open Source PSpipe package.

The rest of the paper is organized as follows: Starting in Sect. 2, we briefly review the statistical framework used by BeyondPlanck and Cosmol oglobe, and we discuss why we believe that these issues will only become increasingly important for all future major cosmology and astrophysical missions. Next, in Sect. 3 we give an overview of various possible productivity tools that might be useful for future experiments, as well as different Open Source licenses. In Sect. 4 we provide an overview of the compilation support facilities implemented for the current software, while in Sect. 5 we summarize our documentation and accessibility efforts. Finally, we conclude in Sect. 6.

2. BeyondPlanck, Cosmol oglobe, and Data Longevity

2.1. Breaking degeneracies through joint analysis of complementary datasets

The fundamental motivation for the BeyondPlanck and Cosmol oglobe projects derives directly from the experiences and insights gained within the Planck project. Towards the end of that project, it became clear that the main limiting factor with respect to constraining large-scale CMB polarization comes neither from instrumental systematics nor astrophysics

2 https://beyondplanck.science
3 https://cosmologlobe.uio.no
4 Currently, the parallelization of Commander is the most effective if applied to relatively small, TB-sized data sets. In this case, 1 TB of raw TOD data requires ~ O(10^6) CPU-hours. For a thorough discussion of the topic, please see Galloway et al. (2023a).
5 https://www.astropy.org/index.html
6 https://openastronomy.org/
7 https://cosmostatistics-initiative.org/
8 https://deepskieslab.com/
9 https://darkmachines.org/
10 https://github.com/cmbant/camb
11 https://cosmologist.info/cosmomc/
12 https://github.com/hpc4cmb/toast
13 https://github.com/fbuster/fbuster
14 https://github.com/healpy/healpy
15 https://github.com/simonsobs/PSpipe
Fig. 1.—(Top row) Stokes $Q$ difference map between the 30 GHz Planck 2018 map and the $K$-band 9-year WMAP map, smoothed to a common resolution of 3° FWHM, and the latter has been scaled by a factor of 0.495 to account for different center frequencies; see Gjerløw et al. (2023) for further discussion. (Middle row) WMAP transmission imbalance template (Jarosik et al. 2007). (Bottom row) Planck 30 GHz gain residual template (Planck Collaboration II 2020).

...one cannot robustly characterize the astrophysical sky without knowing the properties of the instrument, and one cannot characterize the instrument without knowing the properties of the astrophysical sky.

One demonstration of this “chicken-and-egg” problem is shown in Fig. 1, reproduced from Gjerløw et al. (2023), where the top panel shows the Stokes $Q$ difference map between Planck 2018 30 GHz (Planck Collaboration II 2020) and WMAP $K$-band (Bennett et al. 2013), after scaling the latter by 0.495 to account for the spectral index of synchrotron emission. Here one can see coherent large-scale patterns that massively dominate over the random noise. The origin of these structures is well understood and can, to a considerable extent, be described by the sum of transmission imbalance uncertainties in WMAP (middle row; Jarosik et al. 2007) and gain uncertainties in Planck (bottom row; Planck Collaboration II 2020). Both the transmission imbalance and the gain estimation rely directly on knowledge about the CMB sky, while estimating the CMB sky relies on knowledge of the transmission imbalance and gain parameters. However, even though their physical origins are well understood, they are still exceedingly difficult to mitigate within each experiment individually, simply because the observation strategy for each experiment leaves them nearly blind to these particular modes. One of the solutions to this problem is to jointly analyze each experiment and use the information in one experiment to break the degeneracies in the other.

Such complementary information need not only come from expensive satellite missions but can also come from less expensive ground-based experiments. One example of this is depicted in Fig. 2, reproduced from Ruud et al. (2015), which shows latitude-averaged polarization differences between the 43 GHz QUIET map and the corresponding 9-year WMAP (red curve) and Planck 2015 (blue curve) maps. In this case, one can see an excess in Planck with respect to QUIET outside $|b| < 1^\circ$, while QUIET and WMAP agree well. The most likely origin of this excess is bandpass-induced temperature-to-polarization leakage (Ruud et al. 2015; Svalheim et al. 2023a) in the Planck map at the level of 0.2% (dotted line), which is fully consistent with the quoted systematic error of this channel of <1% (Planck Collaboration III 2016). To reduce this systematic uncertainty below that achievable by Planck alone, additional external information is required, and the deep and highly cross-linked Galactic plane measurements made by QUIET are precisely what is needed for this.

These are only two relevant examples, and many more could be listed. Nevertheless, such examples motivate our contention that in order to break instrumental and astrophys-
ical degeneracies, all free parameters should be optimized jointly while simultaneously exploiting as many state-of-the-art complimentary datasets as possible. As such, the analysis problem should be solved globally, both in a statistical and a research community sense.

2.2. The BeyondPlanck data model and posterior distribution

As a first proof-of-concept of this global analysis approach, the BeyondPlanck collaboration (BeyondPlanck 2023) was formed with the explicit goal of re-analyzing the Planck LFI measurements. This data set represents a significant, but manageable challenge in terms of data volume and systematics. Also, building on the experiences gained through the Planck project, we chose to adopt standard Bayesian parameter estimation techniques for our computer codes because of their unique flexibility and fidelity in terms of systematic error propagation. In particular, in the interest of saving costs and development time, we chose the CMB Gibbs sampler called Commander (Eriksen et al. 2004, 2008; Seljebotn et al. 2019) as our starting point, which formed a cornerstone in the Planck data analysis (Planck Collaboration IV 2018; Planck Collaboration V 2020; Planck Collaboration VI 2020).

The most crucial component in any Bayesian analysis is a parametric model for the data, which may typically take the following symbolic form,

$$\tilde{d} = \tilde{s}(\omega) + \tilde{n},$$

where $\tilde{d}$ denotes a given dataset, $\tilde{s}(\omega)$ is a signal model with free parameters $\omega$, and $\tilde{n}$ is noise. The posterior distribution, which quantifies the probability distribution of $\omega$ as constrained by $\tilde{d}$, is given by Bayes’ theorem,

$$P(\omega | \tilde{d}) = \frac{P(\tilde{d} | \omega)P(\omega)}{P(\tilde{d})} \propto \mathcal{L}(\omega)P(\omega),$$

where $\mathcal{L}(\omega) \equiv P(\tilde{d} | \omega)$ is called the likelihood, and $P(\omega)$ is called the prior; $P(\tilde{d})$ is a normalization constant that is irrelevant for our purposes. The likelihood quantifies the constraining power of the actual data, while the prior summarizes our pre-existing knowledge regarding $\omega$ before the analysis.

For the Planck LFI analysis that is presented in a series of companion papers, we have adopted a parametric model that takes the following form,

$$d_{\text{st}} = g_{\text{st}}P_{\text{tp},\text{st}} \left[ B^\text{symm}_{\text{pp}} \sum_c M_{\text{c}}(\beta_p, \Delta_{\text{hp}}) d_p + B^\text{asymm}_{\text{pp}} (s^\text{orb} + s^\text{fsl}) \right] + s_j^{\text{fsl}} + n_j^{\text{corr}} + n_j^w,$$

where $\Delta_{\text{hp}}$ denotes a given dataset, $\tilde{s}(\omega)$ is a signal model with free parameters $\omega$, and $\tilde{n}$ is noise. The posterior distribution, which quantifies the probability distribution of $\omega$ as constrained by $\tilde{d}$, is given by Bayes’ theorem,

$$P(\omega | \tilde{d}) = \frac{P(\tilde{d} | \omega)P(\omega)}{P(\tilde{d})} \propto \mathcal{L}(\omega)P(\omega),$$

where $\mathcal{L}(\omega) \equiv P(\tilde{d} | \omega)$ is called the likelihood, and $P(\omega)$ is called the prior; $P(\tilde{d})$ is a normalization constant that is irrelevant for our purposes. The likelihood quantifies the constraining power of the actual data, while the prior summarizes our pre-existing knowledge regarding $\omega$ before the analysis.

For the purposes of the current paper, the specific meaning of each symbol is irrelevant, and we, therefore, refer the interested reader to Sect. 7 in BeyondPlanck (2023) for complete details. Here it is sufficient to note that this expression represents an explicit parametric model of both the instrument, as quantified by $\{g, P, B, \Delta_{\text{hp}}, s^{\text{orb}}, s^{\text{fsl}}, n^{\text{corr}}\}$, and the astrophysical sky as expressed by the sum over components $c$, which for BeyondPlanck includes CMB, synchrotron, free-free, spinning and thermal dust emission, and compact sources.

It is important to note that this model is far richer than what Planck LFI is able to constrain on its own. Simply by counting degrees of freedom alone, we immediately note that the sky model has five free component amplitude parameters per pixel, while the LFI data only provide three independent frequencies. Consequently, the model is massively degenerate, and the LFI data must be augmented with external data. This is done in the current BeyondPlanck analysis by including the WMAP 33–61 GHz (Bennett et al. 2013), Planck HFI 353 and 857 GHz (Planck Collaboration III 2020), and Haslam 408 MHz (Haslam et al. 1982) measurements in the form of pixelized frequency maps. The advantage of this is that the model is now reasonably well constrained – but a major disadvantage is that these external pixelized sky maps may be associated with their own systematic errors that may compromise the final results. To fully exploit the strengths of each dataset in breaking degeneracies through joint analysis, one should ultimately start from raw TOD for all involved observations, and properly model all potential systematic effects. This is a main goal of the Cosmoglobe effort.

2.3. Low-level systematics, data longevity, and cost optimization

Whenever the signal-to-noise ratio of a given dataset increases, new systematic effects become important and must be modeled. This general observation also holds true for the CMB community, which currently targets signals at the nanokelvin level; even minuscule effects need to be accounted for at such low signal levels. This directly increases the importance of external data, as no planned experiment is able to measure all relevant effects internally at the required precision. More typically, each experiment focuses on one piece of the entire puzzle that it does particularly well for technological reasons and relies on other experiments to provide information regarding other free model parameters.

At the most basic level, the reason for this optimization is just a matter of cost and complexity. In particular, modern CMB experiments cost so much that it is unacceptable for funding agencies and taxpayers to repeatedly and needlessly measure the same quantities. For example, the ground-based or sub-orbital experiments typically cost at least about $10M and involve 20–50 people, while current and next-generation satellite experiments usually cost hundreds of millions of dollars and involve hundreds of people.

To achieve new transformative results in the future within realistic budget limits, these existing million-euro investments must be optimally leveraged and re-used for all future experiments. For this to be possible, however, it is also vital that the systematic error budgets of the old datasets are consistent with the requirement of the new experiments. Unfortunately, this has traditionally been a prohibitive challenge for one simple reason: Until now, most CMB experiments have primarily published frequency maps or angular power spectra—that are static by nature—as their main products. Once the time-ordered data have been co-added into pixelized maps, it is no longer possible to account for a wide range of low-level systematic uncertainties, but only a very limited number of high-level uncertainties, such as white noise, correlated noise on large angular scales (Bennett et al. 2013; Basyrov et al. 2023), a single absolute calibration factor (Planck Collaboration Int. XLVI 2016; Gjerlow et al. 2023), or symmetrized beam uncertainties (Planck Collaboration V 2020). This significantly limits the use of legacy data for future analyses.

There are two noteworthy exceptions to this rule, though, namely Planck and WMAP. Both published their full uncalibrated time-ordered data as part of their legacy releases.
Hence, the corresponding co-added frequency maps may, at least in principle, be continuously improved as new information and complementary datasets become available. However, it is also important to note that neither Planck nor WMAP released the data analysis pipelines that were used to reduce the data.

That is problematic for at least two reasons. First, from a practical point of view, the lack of functional analysis pipelines makes it very difficult and time-consuming for external scientists to repeat and improve the original analyses. Even more problematic, however, is the fact that most modern data reduction pipelines typically employ a significant number of critical ancillary datasets, for instance, ADC correction tables or far-sidelobe models. Since these are only used during low-level processing, few external researchers ask for them. As a result, they may easily be forgotten during the last stages of the main collaboration work and sometimes even lost when the original production computer systems are discontinued.

We argue in this paper that the optimal – if not only – way to ensure full reproducibility and data longevity is to release a complete and functional data processing pipeline together with the raw data, parameter files, high-level products, and documentation. Furthermore, we also argue that such a complete release should be required and supported in terms of dedicated funding for all future CMB experiments by the respective agencies (ESA, NASA, JAXA, NSF, etc.). This is clearly also in the funding agencies’ own interests, as it guarantees that their investments may be optimally leveraged in future work.

In addition to sharing data, it is also worth noting that sharing analysis tools may lead to cost optimization of any given new experiment. Indeed, establishing common analysis tools across the field will free up analysis funding that can be better spent on understanding the instrument, exploring ground-breaking theories, or deriving novel secondary science. An important pioneering CMB-related example of this is HEALPix (Górski et al. 2005), which both defines a standard pixelization that facilities easy data sharing and comparison across experiments, and provides a wide range of state-of-the-art and user-friendly tools to operate on these data (e.g., Zonca et al. 2019), all published under an Open Source license. In general, common software tools are highly beneficial for the science community, funding agencies, and taxpayers.

2.4. Open Science: From BeyondPlanck to Cosmoglobe

An important goal for the BeyondPlanck project was to develop and publicly release a complete end-to-end analysis pipeline for one of the essential datasets in contemporary CMB cosmology, namely the Planck LFI data (BeyondPlanck 2023). The motivation for this was two-fold. The first aim was to resolve a few notable issues with the LFI data that remained unresolved at the end of the official Planck mission, in particular related to the global estimation of the instrumental gain (Planck Collaboration II 2020; Gjerløw et al. 2023). However, this represents only a first step in a much larger process, as embodied within the Cosmoglobe program, whose goal is to develop a general low-level analysis pipeline that would be applicable to a much more comprehensive range of experiments – legacy, current, and future – and at the same time support joint analysis of these.

The full scope of this project is massive. For this work to succeed in the long term, it must be firmly based on an Open Science foundation: While a small group of dedicated people may be able to re-analyze one experiment (as BeyondPlanck has done for Planck LFI), integrating a wide range of complementary experiments without community contributions is unfeasible for several reasons. First, some important datasets may be proprietary, and the original stakeholders must be leading the analysis for legal reasons alone. Second, the systematic properties of most datasets are quite complicated, and expert knowledge is usually essential to formulate and generalize the data model. Third, the sheer amount of work to be done effectively requires cost-sharing among all interested parties, recognizing the currently constrained funding environment most researchers experience daily.

In general, Cosmoglobe will be a hub for which analysis of both time-ordered and map-domain data from different experiments can be integrated into a single framework. A critical goal of Cosmoglobe is to support scientists working on incorporating the data from their own experiments into the larger Cosmoglobe framework and thereby analyzing the data efficiently, robustly, and economically. For the casual user who might be primarily interested in what the microwave sky looks like at some specified frequency, Cosmoglobe will provide a state-of-the-art and user-friendly sky model. By allowing scientists easy access and configuration of their experiment in this framework, Cosmoglobe will become an integral tool for forecasting and planning for experiments.

With a functional codebase in hand, as demonstrated by the current LFI-based data release, we believe that the time is now right for all interested parties to get involved in this work and extend the framework according to their own needs. We anticipate that such contributions will most typically take one of two forms. The first is stand-alone projects, in which the external user simply downloads the software and data and performs some analysis without input from the greater community. In this case, the only formal obligation for the user is to publish all derived codes under an equally permissive software license as the one used for BeyondPlanck (which in practice means a GNU General Public License (GPL)) and to acknowledge previous work through appropriate referencing.

The second mode of operation is active participation in the Cosmoglobe framework. In this case, an external user or project may request direct expert Cosmoglobe support, for instance, in the form of software development and data analysis assistance. That is then likely to increase the chance of success significantly. In exchange for the support, the external user or project must commit to publicly releasing the underlying data after some proprietary period, and all directly contributing Cosmoglobe collaborators must be offered co-authorship, in accordance with standard scientific practices. Required details can be specified in a Memorandum of Understanding (MoU) between the external party and the relevant Cosmoglobe participants before the work commences. Cosmoglobe is intended to be a platform for initiating and supporting mutually beneficial collaborations.

3. Reproducibility Survey, Tools, and Licensing

We now turn our attention to the practical aspects of how to build an Open Science-based foundation for this work and examine some of the latest developments on reproducibility in science in general. Next, we identify several tools and services that are available online and aim to provide solutions for reproducible science. Finally, we review the most popular licenses used for Open Source development. These issues cover a variety of topics that constitute the current state of the art in reproducibility and Open Science as of 2018–19.
3.1. Open Science development tools per 2018

We collected information regarding available tools that might be useful to strengthen the reproducibility aspects of the project. We found this exercise quite informative and helpful, and we highly recommend future collaborations to conduct similar meta-studies before starting the data analysis work, as it is easy to get swamped with scientific problem solving once the main effort begins. We also note that the field moves very quickly, and the state-of-the-art is likely to be quite different only after a few years.

3.1.1. Workflow definition tools versus integrated software

We first considered the use of so-called “workflow definition tools” to organize the primary data model and Gibbs sampler discussed in Sect. 2.2. Such workflow managers help scientists define and execute a specific set of tasks, implemented by executing local (or sometimes remote) code, scripts, and other sub-workflows. Each component is only responsible for a small fragment of functionality. Therefore many pieces are working together in a pipeline to achieve the ultimate goal of the workflow, performing a useful task.

There have already been attempts at implementing and utilizing such tools in the CMB community. The most well-known example is the ProC workflow manager\(^\text{17}\) developed by the Max Planck Institute of Astrophysics for the Planck mission. Two popular Open Source and general-purpose tools are Taverna\(^\text{18}\) and The Kepler Project\(^\text{19}\).

The main advantage and attraction of such workflow managers is their ability to construct complex, flexible, and reproducible workflows based on well-defined components. At the same time, what makes these managers work is very strict interfaces between the different components. Unfortunately, this strictness adds significant additional burdens on the code developers, both in terms of a steep learning curve to be able to add new features and in terms of restricted flexibility to implement new solutions to unexpected problems; it is difficult to make substantial changes without breaking compatibility with already existing components. A second significant challenge is efficient memory management. Suppose the various pipeline components are written in different programming languages. In this case, one must either resort to data sharing through slow disks or spend great effort on highly non-trivial in-memory communication.

In general, our experience is that general-purpose workflow managers tend to be more practical for well-established and relatively quick routine tasks than for cutting-edge research that relies on high-performance computing. The most critical priority for our Bayesian analysis framework is computational speed, as a factor of six in runtime can make the difference between a two-month runtime (which is painful but doable) and one year (which is prohibitive). Optimal memory and disk management are, therefore, the key. The second most important priority is code flexibility, allowing developers to introduce changes needed to achieve their goals freely.

After careful consideration, we decided to drop the use of workflow managers, as the official Planck Data Processing Centers (DPCs) did, to maintain optimal coding agility and flexibility. However, in contrast to the Planck DPCs, we instead opted for developing the entire analysis pipeline within one single computer program called Commander\(^\text{3}\), to ensure optimal memory management and computational speed (Galloy et al. 2023a). Two important additional advantages of implementing the entire pipeline within a single code are that the whole collaboration naturally develops a common “language” and knowledge base that are helpful to discuss issues more efficiently, and it also minimizes duplication of effort.

3.1.2. Online development services

Another potentially useful class of tools is the so-called “online development services”. These offer the possibility to perform all development work to be done online through the use of general-purpose web applications. Some of the major players in this area that we evaluated were Open Science Framework\(^\text{20}\), Codeocean\(^\text{21}\), and Zenodo\(^\text{22}\).

One of the major advantages of these services is that, by definition, all work is performed online. This facilitates very easy dissemination since results may be published in an Open Science manner literally in real-time. However, our evaluation is that they are also associated with three main disadvantages, mirroring the issues discussed in the previous section. First and foremost, online services typically impose a specific and inflexible work style that may not suit everybody in a large collaboration. Second, they have a significant learning curve that may be off-putting to many scientists with busy schedules. Third, depending on the plans offered by each provider, authors can easily run out of hosting space or online computational time, requiring them to update their accounts.

While this may make financial sense from the side of the hosting companies, we consider this to be a big disadvantage for authors, just for reproducibility purposes alone. A solution like this might make sense for small projects, but the cost can become prohibitive for larger and heavier collaborations.

At their current stage of development, we, therefore, also decided to avoid the use of integrated online development services and instead leave each collaborator to choose their own development environment individually. We also note that most scientists are, by nature, quite independent-minded and do not necessarily respond well to being imposed on a specific development environment. However, if the available tools offered more obvious advantages, the situation might be different, and we definitely recommend future collaborations to perform a similar survey.

3.1.3. Software repositories

One class of software development tools that is critical for a large-scale Open Source effort is efficient revision control systems (RCSs). This allows users to collaborate on the same computer program or scientific paper in real-time with a minimum of synchronization problems and is a cornerstone of modern software development. As noted above, 56% of the user survey respondents already use at least one such system, with Git\(^\text{23}\) being the most popular.

At the beginning of the program, we quickly settled on Git as our main RCS, primarily because it was most widespread in our group, but also because we find that it handles merges and conflicts better than most competitors. The main question was then which (if any) common repository we should use. Three particularly well-known providers are Bitbucket\(^\text{24}\),

\[\text{http://planck.mpa-garching.mpg.de/ProC/}\]
\[\text{https://taverna.incubator.apache.org}\]
\[\text{https://kepler-project.org/}\]
\[\text{http://planck.mpa-garching.mpg.de/ProC/}\]
\[\text{https://taverna.incubator.apache.org}\]
\[\text{https://kepler-project.org/}\]
\[\text{https://osf.io/}\]
\[\text{https://codeocean.com/}\]
\[\text{https://zenodo.org/}\]
\[\text{https://bitbucket.org}\]
GitHub\textsuperscript{24}, and GitLab\textsuperscript{25}.

One advantage of GitLab and Bitbucket is that they offer free private repositories in addition to public ones. This option might make them a better candidate for users who want to start their project as a private repository but switch to a fully public repository later on, closer to publication time. In addition, all three offer a full suite of online development tools, including bug/issues management, wiki pages, file hosting capabilities, and API access to hosted files.

Initially, we adopted GitLab as our main provider, primarily because it allows code to be run remotely on their web hosts. In addition, we considered that it might be helpful for small tasks, such as implementing online tools and calculators or automatically compiling paper drafts after each submission. However, it is important to note that this feature is only free for limited usage. Therefore, we have concluded it was not as useful as initially anticipated. Consequently, halfway through the project, we have switched to GitHub for our central software repository, simply because most people in our community already have accounts there and to avoid overhead by maintaining two separate accounts for most users.

### 3.1.4. Open Source licenses

When working in an Open Science setting, it is vital to protect the investments and interests of the various contributors and users. A critical aspect of this is licensing. Today, many Open Source licenses are in active use, and an important task for projects like BeyondPlanck and Cosmolite is to choose the appropriate one for the work at hand. In this section, we provide a brief overview of licenses in the most common use today and discuss which one was chosen for our project, given the basic requirements that (1) our software should be Open Source; (2) all derivatives of this work should remain Open Source; and (3) our license should not contradict the licenses of any dependencies (HEALPix\textsuperscript{26}, FFTW\textsuperscript{27}, etc.).

Although the term Open Source software may be intuitively understood to be freely distributable, modifiable, and shareable code written by a single or a group of programmers, it is, in reality, more complex than it may seem at first glance. Generally speaking, when discussing software licenses, one needs to distinguish between several different aspects and concepts. The first aspect concerns basic distribution. On the most restricted side, proprietary software is considered private property, and users are not allowed to share, study, change, or reverse engineer the provided software. A variation of this is called freeware; in this case, the original software developer retains all rights, and the only difference is that end-users do not need to pay for the basic usage of a given program. Source available software is software that allows users to view the source code but does not necessarily give the right to distribute, modify and/or install it on their machines. One example of such a license is the Commons Clause License\textsuperscript{28}, which prohibits users from selling the software. Because of such restrictions, source available licenses are generally not considered to be Open Source. Next, Public Domain software or “unlicensed” software is software that waives all the rights of copyright, trademark, or patent. Such software belongs to the “public” that uses it, and it can be freely distributed, modified, and/or sold without attribution to anyone. Examples of such licenses are Creative Commons (CC0) and Unlicense. During the course of history, experts have been arguing whether this type of license should be considered Open Source or not. Indeed, some argue that the fundamental rights of free and Open Source software are not guaranteed\textsuperscript{29} since the uncopyrighted software may be a subject to restrictions depending, e.g., on the laws of the particular country. Some are going as far as to claim that Public Domain is not at all an appropriate license\textsuperscript{30} for computer software. Because of these disagreements, we also do not consider this license to be a “proper” Open Source license in the present work.

Moving on to what is considered proper Open Source software, free software (FS), as defined by the Free Software Foundation\textsuperscript{31} (FSF), is “software that gives its users the freedom to run, copy, distribute, study, change and improve the software”. According to a formal definition, the software is not considered free if it does not respect the following four essential freedoms:

- **Freedom 0:** The freedom to run the program for any purpose.
- **Freedom 1:** The freedom to study how the program works, and change it so it does your computing as you wish. Access to the source code is a precondition for this.
- **Freedom 2:** The freedom to redistribute copies so you can help others.
- **Freedom 3:** The freedom to distribute copies of your modified versions to others. By doing this you can give the whole community a chance to benefit from your changes. Access to the source code is a precondition for this.

Finally, Open Source licenses are defined by the Open Source Initiative\textsuperscript{33} (OSI) and include licenses that “allow the software to be freely used, modified, and shared”, and comply with ten distinctive criteria\textsuperscript{34} that concern (1) free redistribution; (2) source code; (3) derived works; (4) integrity of the author’s source code; (5) no discrimination against persons or groups; (6) no discrimination against fields of endeavor; (7) distribution of license; (8) the license must not be specific to a product; (9) the license must not restrict other software; and (10) the license must be technology-neutral.

Both FS and OSI are considered to be Open Source with only subtle differences.\textsuperscript{35} While FS is focused on the user’s rights to use, modify and share the program, OSI is focused on the source code being open with unrestricted community driven development.\textsuperscript{36} Since the main goal of the Cosmolite project is to build a community around a common source code, this strongly suggests that the OSI definition is most suitable for our purposes. However, looking at OSI’s list of

\textsuperscript{24} https://github.com
\textsuperscript{25} https://about.gitlab.com/
\textsuperscript{26} http://healpix.sourceforge.net or https://healpix.sourceforge.io
\textsuperscript{27} https://www.fftw.org
\textsuperscript{28} https://commonsclause.com/
\textsuperscript{29} For more details, see, e.g., the “Public Domain Is Not Open Source” article: https://opensource.org/node/878
\textsuperscript{30} Lawyer Lorence Rosen has written the essay titled “Why the public domain isn’t a license” — faced with strong opposition, he has accepted that CC0 can be considered Open Source.
\textsuperscript{31} https://www.fsf.org/
\textsuperscript{32} https://www.gnu.org/philosophy/free-sw.html
\textsuperscript{33} https://opensource.org/licenses
\textsuperscript{34} https://opensource.org/osd
\textsuperscript{35} These are more philosophical in nature. As Richard Stallman, the founder of GNU Project and FSF, stated: “The term ‘open source’ software is used by some people to mean more or less the same category as free software... The differences in extension of the category are small: nearly all free software is open source, and nearly all open source software is free.”
\textsuperscript{36} https://opensource.org/about
Fig. 3. — Licensing diagram for Commander and its dependencies, ordered from left to right according to increasingly specific licenses. Circles indicate libraries and codes, while rectangles show the licenses under which the particular library was issued. The dashed line divides the so-called permissive (i.e., licenses that can be combined and used together with proprietary software) and restrictive licenses (i.e., licenses that enforce the source code to stay open for general public).

In order to select one of these OSI licenses, it is important to recognize that the Commander source code does not exist in a vacuum but rather depends directly and indirectly on a variety of different libraries, as visualized in Fig. 3. When one chooses the correct license for the project, the list of dependencies must be considered. Then, typically, the most specific one defines what is allowed for the new software. However, this is not always the case. For example, cURL is based on the modified MIT license, but it may or may not be compiled with the support of MbedTLS and LibSSH2 that rely on more complicated licenses. The same applies to, e.g., CFITSIO which requires ZLIB starting from version 4.0.0. A third important example is Commander itself, which may be compiled with Intel Parallel Studio and Intel Math Kernel Library (MKL), which are issued under one of Intel’s proprietary licenses. We do not ship or install this library to any way, and, thus, such a decision relies solely on the user’s judgment.

Our understanding is that as long as one does not explicitly modify the source code of a library issued under a permissive license, the licenses can be used almost interchangeably. Generally, this does not apply to the restrictive ones. However, the GPL licenses are internally compatible as long as it includes a special line that explicitly states that the later version of the license can be used. In practice, this means that if a piece of software is issued under GPLv2 and not GPLv2+, then we cannot use it.

All in all, the license adopted for Commander and Cosmoglobe cannot be more restrictive than the most permissive of these, which is set by the GPL+ license adopted for HEALPix. In principle, the same applies to FFTW3, but if needed, this library could have been replaced with other FFT implementations. In contrast, HEALPix is in practice irreplaceable and therefore determines the license also for the current work. Consequently, our final choice is the GNU General Public License v3, as dictated by the diagram. Of course, for us, this is not only a matter of formality but also of preference; we want this software to be and remain Open Source to protect the interests of everybody involved. Therefore, it is crucial for all future participants and developers of the Cosmoglobe framework to familiarize themselves with this license and determine whether this is acceptable for one’s work and compliant with potential collaboration policies.

4. Compilation Support

The Commander software is primarily intended to be run on Linux-based High-Performance Computing (HPC) clusters with basic Fortran and MPI compilers and libraries available and typically tens to thousands of computing cores. Beyond that, it does not impose any specific constraints on the computing platform, neither in the form of processor architecture (AMD, ARM, Cray, Intel, etc.) nor compilers (GNU, Intel, PGI, etc.). At the same time, the code does depend on many external libraries, including HEALPix, FFTW3, CAMB, and HDF5 for full specification, see the online Commander documentation.

The combination of many dependencies and a rich computing platform heterogeneity can, in general, represent a significant challenge and workload in terms of compilation and can be seriously off-putting to many users. Therefore, it is critical to make this process as simple and user-friendly as possible, and automated build systems play a key role in that work.

Build systems come in various flavors and combinations, which makes it non-trivial to choose one among many. As a result, there is no single “best” build system, but each has its advantages and disadvantages. Therefore, when selecting one specific system for Commander, we have considered seven different aspects listed in order of importance.
1) Free and Open-source: Commander will not be a genuinely Open Source tool if the build system which installs it is itself not free and Open Source.

2) Cross-platform: Although Linux was (and still is) the predominant operating system for modern HPC, there is currently a trend toward a more diverse landscape. In addition, Windows and Macintosh software dominate the PC and laptop market, and these systems are growing rapidly in power and can be used today for productive analysis. Hence, we require that the build system allow us to compile and run Commander on any major operating system, including Linux, Windows, and MacOS.

3) Automation: Many astrophysics departments operate today their own computing cluster. However, experience shows that there is often limited professional support for the installation, tuning, and maintenance of software and libraries. This work is often left to the scientists who want to run the code; Ph.D. students, postdocs, and professors. The installation procedure must therefore be both transparent and easy to use. Furthermore, it should be automated, i.e., the build system should be able to check for the existence of specific Commander dependency, and, if it doesn’t find it on the host system, it should download, verify, compile, and install all missing dependencies, compile Commander itself, and link them all together.

4) Long-term support: While Open Source projects have many advantages in current computing, they also tend to have one fundamental flaw: People tend to abandon them in favor of “newer” and “better” codes. This poses an obvious threat to a large and long-term project such as Cosmoglobe, which will require significant community-wide investments over many years. For this reason, the adopted build system should be mature and supported by a dedicated community. Proven stability is more important than cutting-edge.

5) Multi-language support: The bulk of the Commander codebase consists of Fortran code, but there are many Python scripts and libraries written in the course of the development. In addition, there are also several C++ based modules that need to be compiled together with Commander, and other languages may become useful in the future. Therefore, the tool should have support for multiple languages used simultaneously in one project.

6) Minimal dependencies: The build system should have as few dependencies as possible, and these should ideally either be already present in the system or easy to install from the source. Preferably, it should be a single binary or a piece of software.

7) IDE Integration: While Integrated Development Environment (IDE) support is not a strict requirement, it is certainly a nice bonus feature. In the present day and age, people are using a huge variety of IDEs that can perform syntax highlighting and code checking—having the same features available for the build system gives the programmer an advantage in terms of the code development speed.

With these points in mind, we now provide a survey of possible useful compilation support tools in current use and then describe the implementation chosen for Commander.

4.1. Survey of automatic build systems

4.1.1. Low-level build systems – Make

Make is a “low-level” build automation tool which uses special instruction files — so-called Makefiles — to build and install software from the source code. It has a variety of implementations, with perhaps, the most widespread one being GNU Make which is shipped together with most Linux and Unix distributions. In fact, Commander1 and Commander2 were solely built using Make. Its advantages are numerous: It is a standard Linux and Unix tool; it is widespread, and the majority of the scientific and open source community knows about it; it will not be deprecated in the foreseeable future since it has a solid community of maintainers; it has a support for a variety of languages such as C, C++, Fortran, Java, Python, etc.; it allows nested project structures; and, starting from version 3.0, it allows compilation using multiple processes.

However, it also has a few notable disadvantages. First, Make has a relatively obscure syntax and associated steep learning curve. Second, for large projects, such as Commander, the Makefiles tend to become very long and complex and increasingly hard to maintain. Finally, code compilation requires specific instructions for each particular compiler, OS, and architecture, making it a poor solution for cross-platform development. Despite these shortcomings, Make remains the most widespread build system in use today, and it has a firmly established user community. Taking into account both its flexibility and maturity, we have chosen Make as the primary low-level compilation system for Commander.

4.1.2. High-level build system – CMake

Developed since 1999 under a BSD-3-Clause license, CMake is a “meta” or “high-level” build system that is used in conjunction with some other “low-level” build environments, for instance Make, Ninja, or Microsoft Visual Studio. CMake may be used to build a software project in a two-step process: First, CMake reads in a series of configuration files written in CMake’s own scripting language, called CMakeLists.txt, and uses these to automatically produce a complete low-level build system configuration (e.g., Makefiles). Second, these files are used by the low-level native generator (e.g., Make) to actually compile and install the project.

CMake allows for flexible project structures. For instance, nested directory hierarchies and/or complex library dependencies do not pose a problem, as it can locate a variety of files and executables on the host system. Once such dependencies have been identified, the location data are stored inside a special file called CMakeCache.txt that can be manually tuned before the actual build. In addition, it has the functionality to download, verify, unpack and compile archives of missing libraries that utilize non-CMake build systems. Furthermore, cross-compilation is straightforward since CMake has extensive OS, language, and compiler support. Other important features include, but are not limited to, support for mathematical expressions; string, list, and file manipulation; conditions, loops, functions, and macros; and shell scripting.

Today, CMake is the de facto standard tool for C++ project development, and a variety of Open Source projects use CMake as its build system, including several Commander de-
dependencies such as CFITSIO, FFTW3, and HDF5. Lastly, CMake has good support for IDE integration.

However, despite its many strengths, CMake is not perfect. The syntax has a pretty steep learning curve, and the source code may quickly become cumbersome and difficult to read. Also, there does not seem to be a universal approach, or even strict guidelines, for how to structure CMake code for large and complicated projects. Finally, the documentation is extensive but non-trivial to navigate and read for newcomers.

Based on its prevalence, mature community, rich feature set, and the fact that many Commander dependencies also use CMake, we have chosen this as our primary high-level build system, with Make as the corresponding low-level system. Specific details regarding the Commander CMake configuration is described in Sect. 4.2.

4.1.3. Alternative build systems

This section provides an overview of other competing systems that were explored during the initial phases of the project but ultimately not selected. However, several of these may be attractive candidates for future astrophysics and cosmology Open Source projects.

Ninja is a low-level build system, similar to Make, specifically designed for speed. Like Make, it supports a variety of languages, platforms, compilers, and operating systems and, in fact, is meant to eventually replace Make. The main reason for not choosing Ninja over Make is simply the fact that it was designed to be used in combination with high-level build systems and not on its own. In addition, it is still in active development, and this carries a risk of higher – and unnecessary – development overheads for our purposes. This choice is likely to be revisited in the future when Ninja has proven itself further in terms of stability and user base.

QMake or makemake is a build system created by the Qt Company which automates the creation of Makefiles, similar to CMake. It supports multiple platforms and can produce Makefiles tuned for specific operating systems. Although mostly used for C++ projects, it can incorporate custom compilers (e.g., gfortran), and this allows it to work with Fortran source files. However, it lacks native support for non-C++ languages, a natural alternative to Make build tools, and the ability to incorporate third-party libraries directly into the build.

XMake is a lightweight build system that supports multiple languages, tool-chains, and platforms, and it can compile projects both directly and produce configuration files for low-level build systems such as Make or Ninja. However, native Fortran support was added as recently as July 2020 (in version 2.3.6), well after a system had to be chosen for the current Commander development. It is fast and has many IDE plug-ins.

GNU Autotools is a GNU build system composed of several utility programs that are designed to make source code portable to many Unix-like Operating Systems. It is widely used by many free and Open Source projects, including several astrophysical and cosmology ones. In general, Autotools generate the distribution archive used to build programs. Once users obtain this package, they need to unpack it and run three simple and well-known commands – configure, make and make install – to compile and install the code using the facilities provided by their host systems. Such an approach, in theory, eliminates the need to install Autotools entirely, but, in practice, Linux distributions still have it with (sometimes) multiple versions installed, which adds to the confusion. Furthermore, a major drawback of Autotools is its complexity; it requires much experience and time to develop robust and user-friendly configuration files. For many future projects, we consider CMake to be a more accessible and user-friendly solution.

Scons does not implement a new special-purpose and domain-specific language but rather utilizes specific Python scripts to build the projects. Thus, the only requirement is to have Python installed on the system, and this makes Scons cross-platform by default; any system that runs Python can install Scons using Python’s standard installation frameworks, pip or conda. MIT license, good multi-language support, reliance only on Python, and a rich feature set make it a tool worthy of exploring for new projects. A major shortcoming is that there does not appear to be a simple way of integrating other projects or dependencies into the build.

Waf is another build system solely based on Python. Since SCons inspired Waf, both tools have many similar features: They rely exclusively on Python; are cross-platform; can automatically scan for project dependencies; and have support for multiple languages, including C, C++ and Fortran. However, while SCons is older and therefore is used in more projects and has better documentation, Waf seems to be much faster and provides more user-friendly console output that makes it easier to debug. Additionally, it does not require a separate installation since the tool is designed to be shipped as part of the main project source code. Unfortunately, similar to SCons, there is no easy way to incorporate other projects into the build.

Meson is the last Python-based tool considered here and is the closest CMake competitor we have found so far. It is similar to CMake in many (if not all) aspects, and both are meta-languages that compile the source code in a two-step process. However, while CMake uses Make by default, Meson uses Ninja instead; this makes Meson even faster in some cases. It is also an Open Source, cross-platform tool that supports multiple languages, including Fortran. In addition, nested hierarchies are not a problem, as well as the incorporation of other projects (both Autotools- and CMake-based) into the build.

Fortran Package Manager or simply fpm is a relatively new51 initiative by the Fortran-Lang foundation52 inspired by Cargo, the package manager for the Rust programming language. It is both a build system and a package manager that can build libraries and applications. In addition, it has native support for unit testing and can include other dependencies (e.g., from Git) into the project. While looking very promising, we considered that it was not ready for large-scale production at the time when the current project started. Still, this option should be revisited in the future.

4.2. CMake-based compilation

As discussed above, we have adopted CMake and Make as our high- and low-level build systems. In this section, we provide an overview of the Commander-specific CMake configuration and compilation procedure.

4.2.1. Commander-specific CMake-code organization

51 Alpha version was released on Github in November 25, 2020.
52 https://fortran-lang.github.io/fpm/.
called “out-of-source” build approach, as recommended by the CMake creators. In this organization, the source code and compiled build files are stored in separate locations. In our case, the source code itself is located inside the directory called commander3. In contrast, the binary folder is called build\(^53\), and it is usually created by the user inside the root directory. One advantage of out-of-source compilation is that the users can create whatever amount of build folders they want/require; thus, the same source code tree can be used to produce multiple binaries, corresponding, for instance, to different debug flags or CPU architectures.

All in all, the Commander source code directory structure is visualized in Fig. 4. In this figure, root represents the root folder of the project, created by the original git clone command; cmake contains all CMake related files; commander3 contains all Commander related files; docs contains instructions on how to generate out-of-source documentation; logo contains Commander logos; .gitignore is a git version control file; CMakeLists.txt is the top level CMake configuration file, which serves as the starting point for the compilation process; Makefile is a traditional-style Makefile that may be used to compile Commander3 without CMake; and README.md describes the project on Github.

4.2.2. Commander CMake workflow

The CMake process works as follows. First, the host system is scanned, and the present/missing libraries are registered inside CMakeCache.txt and other auto-produced files. Then, once the configure step is done and the user has issued the build command, CMake downloads, configures, compiles, and installs the missing dependencies and, together with the ones identified as available, it links all libraries to the compiled Commander.

The CMake module that enables this behavior is called ExternalProject, and its primary purpose is to facilitate downloading and installation of dependencies that are not an internal part of the main project. In this way, the Commander dependencies are treated as entirely independent entities. Such isolation allows the build to be performed in the same way on different platforms, with utterly different build settings (e.g., compiler flags) and/or with a completely different build system (e.g., Autotools). Under the hood, it defines the set of so-called targets, each representing a particular step in the build process of an external project. These steps are then collected under a unified name (in our case, a sub-project name), used later in the code. CMake also remembers information about each performed step, which, if executed successfully, will not be repeated. This allows us to compile all dependencies only once for different Commander build types. An essential feature for debugging this process (if and when something fails) is the CMake logs, which are stored in /usr/local/logs\(^54\).

Command-line arguments determine compiler selection during the scan phase. For instance, -DCMAKE_Fortran_COMPILER=ifort tells CMake to use the Intel ifort compiler. Then, for the most common compilers default optimization flags are defined per (sub-)project in a configuration file called

\(^{53}\) It is worth noting that there is nothing special about this name, and the users can name the directory where the CMake build files will be stored in whatever way they prefer. However, the convention is to name it build.

\(^{54}\) The location can be changed by using defined CMAKE_LOG_DIR variable during the configuration process. We refer the interested reader to Commander documentation for further details.
cmake/projects/<project_name>.cmake. When installing this software on a new system with a new, unknown to Commander compiler, these are the configuration files that most likely need to be updated.

Based on the initial system scan and user-specified compilation instructions, CMake proceeds with the following steps for each dependency and for the main Commander source (the two first steps are skipped in the latter case):

**Download:** The project is downloaded via external links in the form of .zip or .tar.gz archives, or directly from Git repositories. We use MD5 hashes whenever possible to ensure that the correct library versions are downloaded.

**Update/Patch:** This step applies potential patches to the downloaded archive or, in the case of Git, brings the project up to date. In cases where we download the release versions of the packages, we skip this step.

**Configure:** This step can use CMake and other build tools alike, depending on the preferences of the authors of the original dependency. In our case, most libraries use Autoconfig scripts and Makefile to compile.

**Build:** In this stage, we use the default build tool as in the rest of the project.

**Install:** The subproject is installed to a local directory specified by the user during the CMake configuration stage. It is worth noting that not all projects (e.g., HEALPix) support an explicit install command. We simply copy the compiled binaries and libraries into the specified directory in these cases.

These steps can either be sequential or parallel. In the former case, each library is built sequentially, while the latter allows some libraries to be built in parallel. This idea is illustrated in Fig. 5. It is important to note that this is not the only way to compile Commander since OpenBLAS can be substituted for, e.g., Intel MKL, which will be detected by CMake if present.

### 4.2.3. Installation regimes

CMake has various build types defined by default that allows for different optimization categories. We are calling these “installation regimes” with four of these currently supported:

**Release:** Builds Commander with the most aggressive optimization flags enabled, tuned for each specific compiler and platform. At the time of writing this paper, only Intel and GNU compilers were supported.

**Debug:** Builds the Commander executable without any optimization, but with debug symbols.

**RelWithDebInfo:** (“Release With Debug Information”). A compromise between the two above, building the Commander binary with less aggressive optimizations and with debug symbols.

**MinSizeRel:** (“Minimal Size Release”). Builds the Commander executable with optimizations that do not increase object code size. However, as the current software...
targets HPCs with ample disk space, this feature is not used frequently, and it is also accordingly not thoroughly tested.

While we have defined RelWithDebInfo to be the default one, the installation regime is determined by the user and his/her needs and can be changed via specifying CMAKE_BUILD_TYPE variable in the command line. In general, all external libraries are produced in Release format with all optimization flags enabled. This can, however, be changed on a case-by-case basis by editing the CMake source files mentioned above.

5. DOCUMENTATION, QUICKSTART GUIDE, AND ACCESSIBILITY TOOLS

For an Open Science project to succeed and continue to grow, making the source code and the data open to the general public is not sufficient. It is also critical that the framework is easy to use and adapt from the user’s perspective. Therefore, in this section, we provide a QuickStart guide to the Commander documentation and compilation, as well as discuss some valuable tools that make it easy for new users to get “up-to-speed” quickly. We note, however, that this is a continuous work-in-progress; thus, the section is only intended to give a snapshot of the situation at the time of publication.

While the CosmoGlobe framework is designed to simultaneously handle data from different experiments, it is helpful to consider the specific BeyondPlanck pre-processing and analysis pipeline in greater detail, as this will typically serve as a point of reference for most users, whether they want to reproduce the LFI work or generalize the framework to other datasets. In the following, we, therefore, give an overview of the BeyondPlanck installation procedure, but note that most of these steps will be identical for any Commander-based analysis.

5.1. Online documentation

The documentation for the BeyondPlanck pipeline and Commander are currently available on the Commander documentation page of the official CosmoGlobe GitHub repository. It consists of five main sections, namely (1) Overview (2) QuickStart and installation guide; (3) The Commander parameter file; (4) File formats; and (5) Frequently asked questions.

Due to the dynamic nature of the Commander and CosmoGlobe projects, this documentation will continually evolve with the addition of new features or experimental datasets. Hence, active participation by the community is essential for its maintenance and expansion. Relatedly, it is also worth noting that because of the high Commander development rate, sometimes developers forget to document newly added parameters, and the documentation then becomes outdated. When this happens, the code may request parameters that are not explicitly mentioned anywhere. In these cases, we strongly recommend that the external user notifies the core developers by opening a GitHub issue – or, better yet, corrects the documentation and submits the improved version in the form of a pull request.

5.2. BeyondPlanck QuickStart guide

In the ideal case, installing the BeyondPlanck analysis framework can be done in four simple steps:

> git clone https://github.com/CosmoGlobe/Commander.git

The first line downloads the Commander from the official Git repository, while the second line creates the aforementioned build directory in which compiled binaries and libraries will be stored. The third line collects information regarding the system and auto-generates Makefiles inside build. Finally, the last line downloads any potentially missing external dependencies and compiles both these and the main source code. The whole process typically takes less than 10 minutes. We have used Intel compilers in this example, but GNU ones have also been successfully tested.

Once Commander is installed, the second step is to download the required input data. The number of different files required for a complete BeyondPlanck run can be somewhat intimidating at first sight. To solve the problem, we have implemented a small Python utility called bp that helps new users to download all required data with a single command:

> bp download all

This creates a complete directory structure with all required inputs, which amounts to more than 1 TB of data. With a modest download speed of 10 MB/s, this can take some time before completion. The tool also supports downloading individual sub-directories in case the user only requires a subset of the total data.

The third step is to edit the Commander parameter file. As described by Galloway et al. (2023a) and in the Commander documentation, this is a human-readable ASCII file. It is the step with the steepest learning curve in the process, as the number of Commander parameters is quite significant, and a typical parameter file spans several thousands of lines. To address the issue, we have enabled support for the nested include statements allowing for rarely used parameters to be hidden from the user. The downside of this approach is that the special environment variable should be defined in the user’s shell for everything to work. Even more so, although very helpful in most cases, such abstraction can still lead to difficult-to-debug errors and become a potential time spender since it requires considerable experience to debug Commander parameter files efficiently. A good strategy, in this case, is to start with a well-tested case (such as the final BeyondPlanck parameter file) and only make a few changes between each test run, carefully visually inspecting all outputs at each step while gradually building intuition regarding the code outputs.

The fourth and final step is to actually run the code, which is typically done through an MPI runtime environment:

> mpirun -n [ncore] path/to/Commander param.txt

56 After installing Commander, the user needs to update the shell to point out the location of the recently installed HEALPix library. This is done by exporting the HEALPix variable inside .bashrc (or similar file).

57 It is called COMMANDER_PARAMS_DEFAULT, and it should point to the <commander_root>/commander3/parameter_files/defaults inside .bashrc (or other shell files if applicable.)
The runtime for a given job varies wildly depending on the parameter file and computing facilities. Still, for the default BeyondPlanc parameter file and a 128-core cluster, it takes about 1 hour and 40 minutes to produce one single sample (Galloway et al. 2023a). For a full Monte Carlo posterior exploration that requires thousands of samples, the end-to-end wall-time is typically on the order of months.

This QuickStart guide represents the ideal case where everything works out of the box. At the time of writing this paper, we estimated that the framework had been successfully installed on at least 20 independent computer systems – and, unfortunately, the default process outlined above worked without modifications in no more than half of these. In the remaining cases, various issues popped up because of compiler idiosyncrasies, missing (or wrong version of) system utilities, insufficient user permissions or disk space, etc. To solve such issues when they arise and improve the current tools, it is vital to have a deeper understanding of all parts of the process, which is the main topic of the rest of the section.

5.3. BeyondPlanc pre-processing and initialization

To understand the whole BeyondPlanc analysis process, it is helpful to take a high-level look at the entire pipeline. This is schematically illustrated in Fig. 6. The heart of this pipeline is the Commander3 execution, discussed in the previous section and illustrated here by the rightmost analysis loop. This is where the actual posterior sampling takes place (see Sect. 2.2), and it is implemented in terms of a ~60,000 line Fortran code, as described by Galloway et al. (2023a).

However, Commander requires a significant number of input data objects in order to run, as illustrated by the various small boxes to the left in the figure. These include (1) the raw Planck LFI Level-1 data (light blue box; Planck Collaboration II 2020); (2) a so-called “instrument file” (orange box); (3) external and ancillary data that need no pre-processing (white boxes); and (4) external or ancillary data that do need slight pre-processing to conform with Commander conventions (colored boxes).

Going through these in order of low to high complexity, the white boxes represent external sky maps and ancillary data that may be used directly in their original forms. These include the frequency maps from Planck HFI, WMAP, and Haslam 408 MHz, as well as beam files and the Planck LFI Reduced Instrument Model (RIMO). In many cases, these may be simply downloaded directly from external repositories, such as the Planck Legacy Archive58 or LAMBDA59, and inserted into Commander in their original form.

However, some information needs to be slightly pre-processed to match the format expected by the Commander. One example is the white noise specification per frequency band (yellow boxes), for which Commander expects the user to provide a standard deviation per pixel, whereas the official Planck products provide a per-pixel 3 × 3 covariance matrix. As such, the external user needs to reformat the Planck format into the Commander format (or, better yet, implement support for the native Planck format directly into Commander, and submit a Git pull request).

Another important example is masks (green boxes), which are used at various stages during the Commander processing. These may be defined differently whether one is considering correlated noise, gain, bandpass, foreground, or CMB estimation (e.g., Ihle et al. 2023; Gjerløw et al. 2023; Colombo et al. 2023; Paradiso et al. 2023; Andersen et al. 2023; Svalheim et al. 2023b). These masks are typically based both on external sky maps (e.g., Planck HFI or WMAP) and internal results from a previous Commander iteration (e.g., \( \chi^2 \) maps), and properly optimizing these is an important (and non-trivial) task for any Commander user.

The third data collection box represents the so-called Commander instrument file. This plays a similar role as the RIMO in Planck and contains detailed instrument information for a given frequency channel and detector. This includes ob-

58 https://pla.esac.esa.int/
59 https://lambda.gsfc.nasa.gov
jects that are general for all detectors, such as bandpasses and beams (Galloway et al. 2023b; Svalheim et al. 2023a), but also instrument-specific objects such as ADC correction tables (Herman et al. 2022).

However, the most significant and crucial pre-processing step is the preparation of the actual raw time-ordered data, as indicated by the three “Preprocess” stages. These data are stored in compressed HDF5 files (Galloway et al. 2023a), and include everything from raw detector readouts, pointing, flags, and satellite velocity to initial gain and noise estimates per Planck pointing period.

To improve both user-friendliness and reproducibility in each of the above steps, it is useful to define scripts that perform all these tasks for the user. Within the Commander repository, we have therefore provided a series of (primarily Python) scripts that perform each of these operations, from mask and instrument file generation to full Level-1 data processing. These are intended to serve as useful starting points for users who seek to reproduce the current BeyondPlanck LFI processing and for users who want to analyze a completely new dataset with the same framework. If so, it would be greatly appreciated if the new scripts are also committed to the existing repository as part of the community-driven Open Source activities.

Before concluding this section, it is worth noting that Commander has, in general, very few means of validating a given input data product. If, say, some instrument specification or compressed HDF files are inter-mixed, there is no automatic way for the algorithm to discover this except through visual inspection of the final results and goodness-of-fit statistics. Furthermore, such parameter file errors are likely among the most common and time-consuming errors made when running this code. For most analyses, it is, therefore, useful to start with the set of well-tested parameter and input files provided in the Commander repository (Galloway et al. 2023a), which includes individual parameter files for a wide range of common datasets (Planck LFI and HFI, WMAP, Haslam 408 MHz, etc.) and astrophysical components (CMB, synchrotron, thermal dust emission, etc.). These may be used as “building blocks” when constructing a new analysis configuration.

5.4. Docker environment for user-friendly data access and code exploration

We provide a precompiled Ubuntu-based Docker image for users who are not interested in computationally expensive analyses like BeyondPlanck but simply want to run Commander on a small dataset for which computational efficiency is not paramount. This self-contained operating-system-level virtual container can be run on any OS (Mac, Windows, Linux, etc.), and all dependencies are maintained within the Docker image itself. Running Commander in this mode amounts to one single command line:

```bash
> docker run -it
-v {input_dir}:/input
-v {output_dir}:/output
registry.gitlab.com/beyondplanck/r13y-helper/cm3
commander3 {parameter file}
```

where `input_dir` is a directory that contains all required input data, and `output_dir` is an empty directory that will contain the results.

We emphasize, however, that the binary provided in this Docker image is not optimized for any processor type. Therefore, it is computationally less efficient than a natively compiled version. Also, debugging this version is non-trivial since it may be challenging to recompile the binary with different debug flags or source code changes.

6. Discussion

The successes achieved in modern CMB cosmology during the last decades are a solid testament to the ingenuity and dedication of thousands of instrumentalists, observers, data analysts, and theorists. However, these same successes are also a direct product of long-standing and invaluable financial support from ordinary taxpayers. A typical CMB satellite mission costs several hundreds of millions of dollars, euros, or yen. At the same time, a ground-based and sub-orbital experiment typically cost from a few to many tens of millions of dollars – and the massive next-generation ground-based CMB-S4 experiment is anticipated to cost $600 M.

With steadily rising costs for each generation of experiments, it also becomes even more critical to optimally leverage the investments already made from previous efforts. For instance, it makes very little sense for future experiments to reproduce the temperature sensitivity of Planck. Instead, they should aim to provide complementary information that may be combined with the Planck measurements, typically in polarization or on small angular scales. Likewise, it makes very little sense for a future satellite mission, such as LiteBIRD, to measure small angular scales from space when this can be done much more economically from the ground at a much lower cost, for instance, with CMB-S4.

In this paper, we argue that the most efficient way to move forward as a field is precisely through an integrated joint global analysis of complementary datasets. However, several prerequisites must be in place for this to be possible. First and foremost, researchers in the various teams actually need to have physical access to data from other experiments. Traditionally, this has been achieved through dedicated “Memoranda of Understanding” (MoUs) between pairs of collaborations; the ground-breaking joint analysis of Planck and BICEP2 is a well-known example of this (BICEP2/Keck Array and Planck Collaborations 2015). While this works reasonably well for limited two-party cases, we believe that this approach is impractical for future work when many datasets must be involved in the same analysis to obtain optimal results, for instance, when combining proprietary data from LiteBIRD (Sugai et al. 2020), CMB-S4 (Abazajian et al. 2019), C-BASS (Jones et al. 2018), QUIJOTE (Génova-Santos et al. 2015), and PASIPHAE (Tassis et al. 2018) with public data from Planck and WMAP. Rather, we believe the time is overdue to fundamentally change how the CMB field works and move to a fully Open Science mode of operation where both raw data and end-to-end analysis methods are shared between experiments and research groups. This also guarantees that taxpayers and funding agencies get maximum value for money, as it vastly increases the longevity of any given dataset. Hence, the funding agencies should require an Open Source release of raw data, analysis tools, and high-level products for any future experiment.

A second prerequisite is using practical analysis methods to exploit the information stored in these complementary datasets. Establishing one set of such common tools is the primary goal of the BeyondPlanck and Cosmoglobe efforts. Our implementation is based on well-established Bayesian parameter estimation techniques and builds directly on the Commander code developed for and used by Planck. This
software is released under a permissive Open Source GPL license, ensuring that any researchers may use, generalize, and modify the code as they see fit (BeyondPlanck 2023; Galloway et al. 2023a). The only requirement is that these modified versions must also be released under an equally permissive license, ensuring that other scientists may then also benefit from the extended work.

However, it is still not sufficient that the data and analysis codes are publicly available. They must also be accessible, and that is the main topic of the current paper: For other scientists to be able to leverage this work in practice, the software must be appropriately documented, and it must be straightforward to install on a range of different computer systems. These practical aspects may seem somewhat mundane compared to the more spectacular topics typically addressed in astrophysics and cosmology papers—but they are no less important in this era of mega-science. These aspects also require significant dedicated resources to be successful, and BeyondPlanck dedicated as much as 20% of its budget (or 300 k€) to this work. On the other hand, these resources do not scale linearly with the total budget size. However, we still strongly recommend future experiments allocate significant funding for reproducibility and Open Source dissemination in their proposal budgets. We hope that the current paper may serve as a valuable and thought-provoking starting point for future large experiments and collaborations that are likely to face similar issues.

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