

CppTransport: a platform to automate calculation of inflationary correlation functions

David Seery

Astronomy Centre, University of Sussex, Falmer, Brighton BN1 9QH, UK

E-mail: D.Seery@sussex.ac.uk

Abstract. CppTransport is a numerical platform that can automatically generate and solve the evolution equations for the 2- and 3-point correlation functions (in field space and for the curvature perturbation ζ) for any inflationary model with canonical kinetic terms. It makes no approximations beyond the applicability of tree-level perturbation theory. Given an input Lagrangian, CppTransport performs symbolic calculations to determine the ‘Feynman rules’ of the model and generates efficient C++ to integrate the correlation functions of interest. It includes a visualization suite that automates extraction of observable quantities from the raw n -point functions and generates high quality plots with minimal manual intervention. It is intended to be used as a collaborative platform, promoting the rapid investigation of models and systematizing their comparison with observation. This guide describes how to install and use the system, and illustrates its use through some simple examples.



Contents

1	Introduction	2
1.1	Automated calculation of inflationary correlation functions	3
1.2	The CppTransport platform	4
1.3	Summary of features	7
1.4	Notation and conventions	8
2	Installation	9
2.1	Minimum requirements	9
2.2	Downloading the CppTransport platform	11
2.3	Building the translator and installing the runtime system	11
2.3.1	Installing dependencies on OS X	11
2.3.2	Installing dependencies on Ubuntu 16.04	13
2.4	Building the translator	13
2.5	Configuring your environment	14
3	The translator: generating custom code for a specific model	17
3.1	Adding model metadata	18
3.2	Specifying a template	20
3.3	Choosing a stepper	20
3.4	Adding author metadata	22
3.5	Specifying field content and Lagrangian parameters	23
3.6	Specifying the Lagrangian	23
3.7	Running the translator and producing output	25
3.8	Using the code generation options	27
4	Building and running an integration task	31
4.1	Coupling a model to the runtime system	31
4.2	Translate and build using a CMake script	34
4.3	Adding an integration task	37
4.4	Running tasks	42
4.4.1	Running executables under MPI and creating a repository	43
4.4.2	Examining the repository wavenumber configuration databases	46
4.4.3	Launch and track tasks from the command line	50
4.5	What happens while an integration task is in progress	52
4.6	Using checkpoints and recovery to minimize data loss	54
4.7	How is the integration time spent?	57
4.7.1	Using HTML reports to analyse integration performance	57
4.7.2	Generating a Gantt chart of worker activity	60
4.8	Using the SQLite data container	63
4.8.1	Table definitions	63
4.8.2	Strict consistency checking	67

5	Options for integration tasks	67
5.1	General options	67
5.2	Two-point function tasks	70
5.3	Three-point function tasks	70
5.3.1	Cubic (k_1, k_2, k_3) mesh	70
5.3.2	Fergusson–Shellard (k_t, α, β) mesh	71
5.3.3	Specifying a storage policy	72
5.3.4	Specifying a triangle policy	73
6	Adding postintegration tasks	74
6.1	ζ tasks for the two- and three-point functions	75
6.2	Applying tags to control which content groups are used	76
6.3	Paired ζ tasks	77
6.4	Using ζ SQLite data containers	78
6.4.1	ζ two-point function tasks	78
6.4.2	ζ three-point function tasks	79
6.5	Inner-product tasks to compute f_{NL} -like amplitudes	81
6.5.1	The standard templates	82
6.5.2	Building an inner-product task	82
6.5.3	Example: Using the SQLite data container to produce a plot	84
7	Generating derived products using output tasks	87
7.1	Selecting which data to plot using SQL query objects	87
7.2	Example: plotting the evolution of the background fields	88
7.3	Derived products: plots and tables	93
7.3.1	Standard options	93
7.3.2	Plot-specific options	95
7.3.3	Table-specific options	97
7.4	Available derived lines	98
7.4.1	Standard options	98
7.4.2	Options for 2-point correlation functions	100
7.4.3	Options for 3-point correlation functions	100
7.4.4	Time series	101
7.4.5	Wavenumber series	105
7.4.6	Integration cost analysis	107
7.5	Enabling or disabling indices using an <code>index_selector<></code>	108
7.6	Examples: double quadratic inflation	108
7.6.1	ζ power spectrum	109
7.6.2	Spectral index for ζ power spectrum	109
7.6.3	Reduced bispectrum on equilateral configurations	110
7.6.4	Spectral index of reduced bispectrum on equilateral configurations	110
7.6.5	Squeezing dependence of reduced bispectrum: isosceles triangles	111
7.6.6	Time evolution of 3pf correlation functions	112
7.6.7	f_{NL} amplitude	114

8	Managing repositories	114
8.1	Managing records	114
8.1.1	Specifying which objects to modify	116
8.1.2	Adding and removing tags	116
8.1.3	Adding and removing notes	117
8.1.4	Deleting content groups	117
8.1.5	Lock and unlock groups	117
8.2	Summary of command-line options	117
9	Acknowledgments	120
A	Third-party software used by CppTransport	121

1 Introduction

There is now broad agreement that the inflationary scenario [1–6] provides an acceptable framework within which to interpret observations of the very early universe. In this scenario, all structure arises from a primordial distribution of gravitational potential wells laid down by quantum fluctuations during an early phase of accelerated expansion. After inflation the universe is refilled with a sea of cooling radiation, and matter begins to condense within these potential wells. This generates a network of structure inheriting its statistical properties from those of the seed quantum fluctuations. By measuring these properties we can hope to infer something about the microphysical modes whose fluctuations were responsible.

Information about the pattern of correlations visible within our Hubble patch can be extracted from any observable that traces the condensed matter distribution. To determine the viability of some particular inflationary model we must compare these observations with predictions that carefully account for the precise character of quantum fluctuations given the field content, mass scales and coupling constants of the model.

Unfortunately these calculations are challenging. Various approximate schemes to compute a general n -point function are known, but even where these are available they require numerical methods except in special cases. Such schemes typically break the calculation into two pieces: a ‘hard’ contribution—that is, involving comparatively large momenta—characterized by wavenumbers near the scale of the sound horizon $k/a \sim H/c_s$, and a ‘soft’ contribution involving comparatively low wavenumbers $k/a \ll H/c_s$ [7]. The soft contribution can be computed using the classical equations of motion and is normally the only one to be handled exactly. The hard contribution is estimated by assuming all relevant degrees of freedom are massless and non-interacting. A typical example is the δN formula for the equal-time two-point function of the curvature perturbation ζ ,

$$\langle \zeta(\mathbf{k}_1)\zeta(\mathbf{k}_2) \rangle_t = \underbrace{N_\alpha(t, t_*)N_\beta(t, t_*)}_{\text{soft part}} \overbrace{\langle \delta\phi^\alpha(\mathbf{k}_1)\delta\phi^\beta(\mathbf{k}_2) \rangle_{t_*}}^{\text{hard part}}. \quad (1.1)$$

The indices α, β, \dots , label species of scalar field (with summation implied over repeated indices) and the subscript attached to each correlation function denotes its time of evaluation. The times are ordered so that $t \geq t_*$. Taking t_* to label an epoch when $k_1/a = k_2/a \sim H/c_s$ makes $N_\alpha N_\beta$ correspond to the soft piece and the t_* correlation function correspond to the hard piece. This division is entirely analogous to the factorization of hadronic scattering amplitudes into a hard subprocess followed by soft hadronization.

Any scheme of this type will break down if the hard initial condition can not be approximated by the ‘universal’ massless, non-interacting case. In recent years it has been understood that there is a rich phenomenology associated with this possibility, including ‘gelaton-like’ [8] or ‘QSFI-like’ [9–11] effects. With sufficient care these effects can be captured in an approximation scheme such as (1.1), but the approach becomes more complex—and even if this is possible we have only exchanged the problem for computation of the hard component $\langle \dots \rangle_{t_*}$. If this hard component is not universal, then the problem is no easier than calculation with which we started.

A different way in which (1.1) loses its simplicity occurs when there is not a single hard scale, but a number of widely separated scales. For example, this can occur in an n -point

function with $n \geq 3$ where the external wavenumbers \mathbf{k}_i divide into groups characterized by typical magnitudes $\mu_1, \mu_2, \dots, \mu_N$ and $\mu_1 \ll \mu_2 \ll \dots \ll \mu_N$. In this case the factorization in (1.1) becomes more involved [12], and must be modified in a way depending on the precise hierarchy of groups.

Taken together, these difficulties generate a significant overhead for any analysis where accurate predictions of n -point functions are important. The form of this overhead varies from model to model, and even on the range of wavenumbers under consideration. If we choose to pay the overhead and pursue this approach, we encounter three significant obstacles. First, a sizeable investment may be required—due to field-theory calculations of the hard component—before analysis can commence for each new model. Second, because each hard component is model-specific, there may be limited opportunities for economy by re-use. Third, if we implement the hard component of each model individually (perhaps using a range of different analytic or numerical methods), we must painfully test and validate the calculation in each case.

1.1 Automated calculation of inflationary correlation functions

To do better we would prefer a completely general method that could be used to obtain accurate predictions for each n -point function, no matter what mass spectrum is involved or what physical processes contribute to the hard component. Such a method could be used to compute each correlation function directly, without imposing any form of approximation.

The same problem is encountered in any area of physics for which observable predictions depend on the methods of quantum field theory. The paradigmatic example is collider phenomenology, where the goal is to compare theories of beyond-the-Standard-Model physics to collision events recorded at the Large Hadron Collider. In both early universe cosmology and collider phenomenology the challenge is to obtain sufficiently accurate predictions from a diverse and growing range of physical models—and, in principle, the obstacles listed above apply equally in each case. But, in collider phenomenology, the availability of sophisticated tools to *automate* the prediction process has allowed models to be developed and investigated at a remarkable rate. Examples of such tools include [CompHEP/CalcHEP](#) [13–16], [FormCalc](#) [17–20], [HELAC](#) [21, 22], [MadGraph](#) [23–26], [SHERPA](#) [27, 28] and [Whizard](#) [29, 30]. (For an early review of the field, see the *Les Houches Guide to MC Generators* [31].) Their common feature is support for automatic generation of LHC event rates directly from a Lagrangian by mixing three components: (1) symbolic calculations to construct suitable Feynman rules, (2) automatically-generated compiled code to compute individual matrix elements, and (3) Monte Carlo event generators to convert these matrix elements into measurable event rates. This strategy of automation has successfully overcome the difficulties encountered in developing cheap, reliable, model-dependent predictions. In addition, reusable tools bring obvious advantages of simplicity and reproducibility. There have also been indirect benefits. For example, the existence of widely-deployed tools has provided a common language in which to express not only the models but also the elements of their analysis.

In early universe cosmology the available toolbox is substantially less developed. A number of public codes are available to assist computation of the two-point function, including [FieldInf](#) [32–34], [ModeCode](#) and [MultiModeCode](#) [35–38], and [PyFlation](#) [39–41]. But although these codes are *generic*—they can handle any model within a suitable class—they are not *automated* in the sense described above, because expressions for the potential and

its derivatives must be obtained by hand and supplied as subroutines. For the three-point function the situation is more restrictive. Currently the only public code is [BINGO](#) [42, 43] which is limited to single-field canonical models.

Partially, this difference in availability of solvers for the two- and three-point functions has arisen because a direct implementation of the Feynman calculus is not straightforward for n -point functions with $n \geq 3$. In these cases, conversion of formal Feynman integrals into concrete numerical results usually depends on techniques such as Wick rotation that are difficult to implement without an analytic expression for the integrand. Such expressions are seldom available for the time-dependent backgrounds required by cosmology, making integration over the time variable more demanding than for Minkowski-space scattering amplitudes. For this reason it would be considerably more convenient to work with an explicitly real-time formulation.

Recently, Dias et al. described a formulation of field theory with these properties. It can be applied to time-dependent backgrounds more straightforwardly than the traditional machinery of Feynman diagrams [44]. This formulation is based on direct computation of the n -point functions by an evolution or ‘transport’ equation, allowing most of the complexities of field theory to be absorbed into calculation of suitable initial conditions. In inflation these initial conditions *are* universal, *provided* the calculation is started at sufficiently early times where all scalar fields can be approximated as massless. Therefore, obtaining suitable initial conditions becomes a one-time cost, the results of which are easy to compute numerically. The remaining challenge is to implement the evolution equations that bring these initial conditions to the final time of interest. These also have a universal form, parametrized by coefficient matrices that depend only algebraically on the model at hand.

Using this scheme it becomes possible to implement automated calculation of inflationary correlation functions in the same sense as the tools used in collider phenomenology. By performing suitable symbolic calculations we can compute the necessary coefficient matrices for any model, and given knowledge of these matrices it is straightforward to generate specialized code that implements the necessary evolution equations. When compiled this code will take advantage of any opportunities for optimization detected by the compiler, making evaluation of each correlation function as rapid as possible. Finally, by mapping each correlation function over a range of wavenumbers we place ourselves in a position to determine any late-universe observable of interest.

1.2 The CppTransport platform

CppTransport is a platform that implements this prescription. It is the result of three years of development, amounting to roughly 60,000 lines of C++, and consists of three major components:

1. A *translator* (17,000 lines) converts ‘model description files’ into custom C++ implementing suitable evolution equations and initial conditions. The model description file enumerates the field content of the model, lists any parameters required by the Lagrangian, and specifies the inflationary potential. It is also possible to document the model by providing a rich range of metadata.
2. Once this specialized C++ code is available it must be compiled together with a runtime support system to produce a finished product capable of integrating the transport

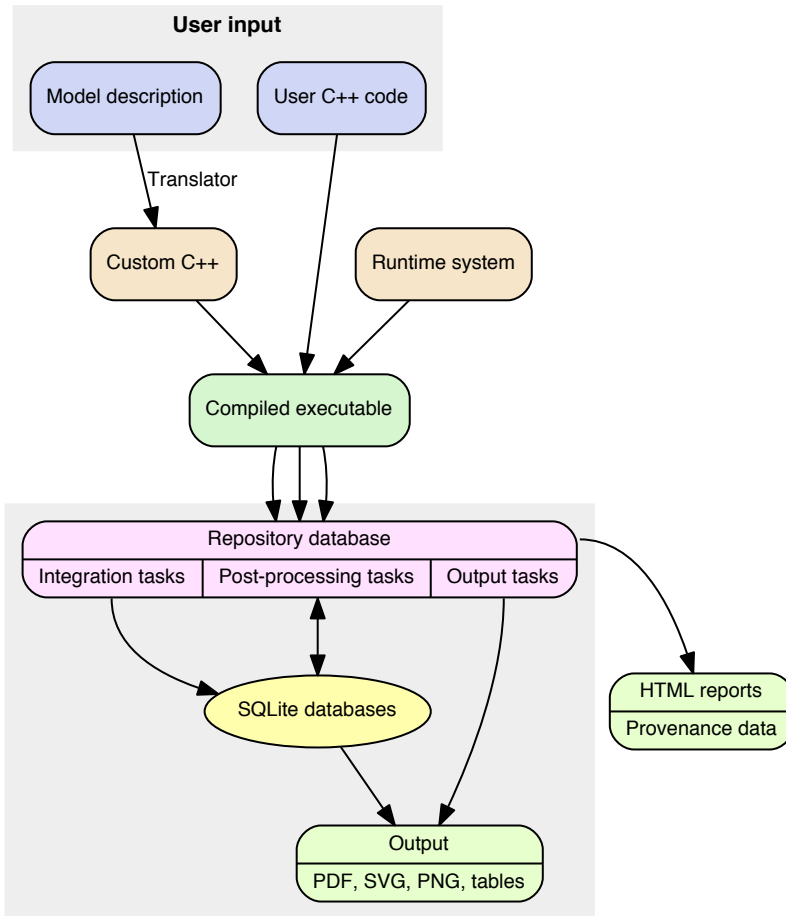


Figure 1. Block diagram showing relation of CppTransport components.

equations and producing correlation functions. The *management system* (29,000 lines) is the largest component in the runtime support and has responsibility for coordinating integration jobs and handling parallelization. It also provides database services.

3. The remaining component is a *visualization and reporting suite* (15,000 lines) that can process the raw integration data to produce observable quantities and present the results as plots or tables. The reporting component generates interactive HTML documents containing these outputs for easy reading or sharing with collaborators.

A block diagram showing the interaction among CppTransport components is given in Fig. 1. To investigate some particular model normally requires the following steps:

1. Produce a suitable model-description file and process it using the CppTransport translator.
2. Produce a short C++ code that couples the runtime system to some number of model implementations produced by the translator—at least one, but up to as many as required. Each implementation is pulled in as a header file via the `#include` directive.

The code can define any number of *integration tasks*, *post-processing tasks* and *output tasks* that describe the work to be done:

- *Integration tasks* associate a single model with a fixed choice for the parameters required by its Lagrangian, and initial conditions for the fields and their derivatives. The task specifies a set of times and configurations (assignments for the wavenumbers \mathbf{k}_i characterizing each correlation function) at which samples should be stored.
 - *Post-processing tasks* act on the output from an integration task or other post-processing task. They are typically used to convert the field-space correlation functions generated by integration tasks into observable quantities, such as the correlation functions of the curvature perturbation ζ . Further post-processing tasks can compute inner products of the ζ three-point function with commonly-defined templates.
 - *Output tasks* draw on the data produced by integration and post-processing tasks to produce summary plots and tables.
3. When compiled and executed, the code writes all details of its tasks into a *repository*—an on-disk database that is used to aggregate information about the tasks and the numerical results they produce.
 4. The runtime system uses the information stored in a repository to produce output for each task on demand. The results are stored in the repository and information about them is collected in its database.
 5. Once predictions for the required correlation functions have been obtained, they can be converted into science outputs:
 - If relatively simple observables are required, such as a prediction of the amplitude or spectral indices for the ζ spectrum or bispectrum, then it may be sufficient to set up an output task to compute these observables directly. The result can be written as a set of publication-ready plots in some suitable format such as PDF, SVG or PNG, or as ASCII-format tables listing numerical values.
 - Output tasks support a limited range of observables. For more complex cases, or to produce plots by hand, the required data can be exported from the databases stored inside the repository.
 CppTransport does not itself provide this functionality, but because its databases are of the industry-standard SQL type there is a wide selection of powerful tools to choose from. Many of these are freely available.
 - To share information about the results that have been generated, CppTransport can produce a report in HTML format suitable for exchanging with collaborators. These reports include a summary analysis of content generated by integration tasks. They also embed the plots and tables produced by output tasks.

1.3 Summary of features

The remainder of this paper will describe these steps in more detail and illustrate how the numerical results they generate can be used to study inflationary models. Acting together, the components of CppTransport provide much more than a bare implementation of the evolution equations for each n -point function. The main features of the platform are:

- Numerical results including **all relevant field-theory effects at tree-level**. The method correctly accounts for a hierarchy of mass scales, interactions among different field species, and correlation or interference effects around the time of horizon exit. It makes no use of approximations such as the separate universe method or the slow-roll expansion.¹
- An **SQL-based workflow** based on the [SQLite](#) database management system,² which CppTransport uses for its data storage. Because SQL is an industry-standard technology there is a rich ecosystem of existing tools that can be used to read SQLite databases and perform real-time SQL queries. This enables powerful GUI-based workflows that allow **scientific exploitation and analysis without extensive programming**.
- A **fully parallelized** MPI-based implementation that scales from laptop-class hardware up to many cores, using **adaptive load-balancing** to keep all cores fed with work. A **transactional design** means it is safe to run multiple jobs simultaneously, and automated **checkpointing and recovery** prevent work being lost in the event of a crash. If modifications are required then the messaging implementation is **automatically instrumented** to assist with debugging and performance optimization.
- Manages the **data lifecycle** by linking each dataset to a repository storing all information about the parameters, initial conditions and sampling points used for the calculation. The repository also collects **metadata about the integration**, such as the type of stepper used and the tolerances applied. Together, this information ensures that each dataset is properly documented and has long-term archival value. (All repository data is stored in human-readable JSON documents in order that this information is accessible, if necessary, without requiring the CppTransport platform.)
- The repository system supports **reproducible research** by providing an unambiguous means to regenerate each dataset, including any products derived from it. This already provides clear benefits at the analysis stage, because it is not possible to confuse when or how each output was generated. But if shared with the community, the information stored in a repository enables every step of an analysis to be audited.

¹In order to obtain accurate estimates of the initial conditions, the slow-roll approximation should be approximately satisfied at the initial time. For more details, see the accompanying technical paper [44]. This also contains a discussion of the validity of the tree-level approximation.

²‘SQL’ is the *Structured Query Language*, a set-based language used nearly universally to express queries acting on the most common ‘relational’ type of database. It is useful because, to extract some subset from a large database, one need only *describe* the subset rather than give an explicit algorithm to search for it; it is the responsibility of the database management system to devise a strategy to read and collate the required records. This is very convenient for scientific purposes because it allows a dataset to be analysed in many different ways, by many different tools, with only modest effort.

- When derived products such as plots or tables are produced, their dependence on existing datasets is recorded. This means that the platform can provide **a detailed provenance for any data product tracked by the repository**. The reporting suite generates HTML documents containing a hyperlinked audit trail summarizing this provenance. Notes can be attached to each repository record, meaning that the report functions as a type of **electronic laboratory notebook**.
- **Leverages standard libraries**, including the [Boost](#) C++ library. Integrations are performed using high-quality steppers taken from [Boost.odeint](#) [45]. These steppers are interchangeable, meaning that they can be customized to suit the model in question. For difficult integrations, very high-order adaptive steppers are available.
- The translator is a full-featured tool in its own right, capable of customizing arbitrary template code for each model using sophisticated replacement rules. It understands a form of Einstein summation convention, making generation of **specialized template code** rapid and convenient.

1.4 Notation and conventions

This document includes examples of computer code written in a variety of languages. To assist in understanding the context of each code block, its background is colour-coded according to the language:

- Shell input or output, blue background: `export PATH=/usr/local/bin:$PATH`
- Configuration files, green background: `input = /usr/local/share/cpptransport`
- C++ source code, yellow background: `class dquad_mpi;`
- Python source code, red background: `def plot:`
- CMake scripts, olive background: `TARGET_LINK_LIBRARIES()`
- SQL code, magenta background: `SELECT * FROM`

CppTransport uses units where $c = \hbar = 1$ but the reduced Planck mass $M_P = (8\pi G)^{-1/2}$ can be set to an arbitrary value.

Each inflationary model can have an arbitrary number of scalar fields. These are all taken to be singlets labelled by indices α, β, \dots , and are written ϕ^α ; their perturbations are $\delta\phi^\alpha$.

CppTransport does not use the slow-roll approximation, and therefore it is necessary to deal separately with the scalar field derivatives $\dot{\phi}^\alpha$ and $\delta\dot{\phi}^\alpha$. We often write these generically as π^α and collect them into a larger set of fields indexed by labels a, b, \dots :

$$X^a = (\phi^\alpha, \pi^\alpha) \quad \text{or} \quad \delta X^a = (\delta\phi^\alpha, \delta\pi^\alpha). \quad (1.2)$$

2 Installation

2.1 Minimum requirements

Compiler.—`CppTransport` is written in modern C++ and requires a relatively recent compiler with support for C++14. It has been confirmed to build correctly with the three major C++ toolchains—`Clang` (including Apple Clang), `gcc` and the `Intel compiler`. The minimum recommended versions are \geq `gcc` 5.0 and \geq `Intel` 16.0. Versions of `gcc` prior to 5.0 have insufficient standard library support, and versions of the `Intel compiler` prior to 16.0 contain bugs that prevent a successful build.³ Any moderately recent version of `Clang` should work correctly.

In the absence of specialized requirements it is usually simplest to build with the default toolchain on your platform. On Linux the default compiler will normally be `gcc`, and for versions of OS X later than 10.7 it will be `Clang`. Testing has shown that there is little to be gained by switching between different compilers, although the `Intel compiler` can give better performance under certain circumstances. Where this occurs it is sometimes possible to obtain the performance improvement by building executables for individual models using the `Intel compiler`, even if the base `CppTransport` system is built with the default system toolchain.⁴

Dependencies.—`CppTransport` is packaged to minimize its pre-requisites and dependencies. Nevertheless, there are inevitably some libraries and tools that must be present before installation can be attempted. These dependencies have been organized by splitting them into two groups. The first group contains those that must be installed system-wide (and therefore may or may not be installable by individual users in a cluster environment), or which are very commonly available from package management systems. The second contains more specialized libraries. `CppTransport` expects dependencies in the first group to be pre-installed by a system administrator, or via a package-management system on a personal computer. (Some examples are discussed below.) This approach uses system resources economically by promoting use of shared libraries. Dependencies in the second group are managed internally and do not require user intervention.

Pre-requisite dependencies.—The dependencies that must be installed prior to building `CppTransport` are:

- **CMake build system.** The build process for `CppTransport` is managed by the `CMake` tool, which is responsible for finding the various libraries and system files needed by `CppTransport`. It is also responsible for downloading and installing those dependencies that `CppTransport` manages internally. Once all resources are available, `CMake` automatically builds and installs the `CppTransport` platform.

`CppTransport` requires `CMake` version 3.0 or later.

- **A working MPI installation.** `CppTransport` uses the standard MPI message-passing system to coordinate parallel calculations. A suitable implementation must therefore

³On Linux, the `Intel compiler` normally depends on the standard library supplied with `gcc`. This means that `gcc` \geq 5.0 should also be available.

⁴This can go wrong if there are binary incompatibilities between compiled code generated by different compilers.

be installed. Any standards-compliant choice should work, including [OpenMPI](#), [MPICH](#) (or its derivatives) or the [Intel MPI](#) libraries.

- **The Boost C++ libraries.** CppTransport uses a suite of C++ libraries called [Boost](#). Most Boost libraries are header-only and do not require shared libraries to be pre-built. However, some do require a build step. Those required by CppTransport are [Date_Time](#), [Filesystem](#), [Log](#), [MPI](#), [ProgramOptions](#), [Random](#), [RegEx](#), [System](#), [Serialization](#), [Thread](#) and [Timer](#).

CppTransport will function with any version of Boost later than 1.56, but is more efficient with version 1.58 or later.

- **The GiNaC computer algebra library.** [GiNaC](#) is a library for performing symbolic computations in C++. It was originally developed as part of the [XLOOPS-GiNaC](#) project to develop an automated 1-loop particle physics code. However, the library itself is independent of any particular application. GiNaC has a further dependence on the [CLN](#) project, but this will be handled automatically if installation is managed by a packaging system.
- **The SQLite database library.** This is almost certain to be installed on every Linux or OS X machine, but some extra developer files may be required.
- **The OpenSSL library.** This is needed to calculate MD5 hashes, which CppTransport uses to uniquely identify models. The MD5 algorithm is used to give consistent results on all platforms.

Typically, some of these dependencies (such as CMake, an MPI implementation, Boost, SQLite, OpenSSL) will already be available in a managed HPC environment such as a compute cluster. All of them are widely packaged for convenient installation on personal machines: they are included in the most common Linux distributions, and are available using the [MacPorts](#) or [Homebrew](#) package-management systems for OS X. CppTransport is agnostic about how these libraries are installed, but unless there are compelling reasons to install in some other way the packaged versions normally represent the most convenient approach.

In addition CppTransport can use certain external programs if they are available, but does not depend on them for its core functionality:

- Using output tasks to generate plots depends on [Python](#) and the [Matplotlib](#) library. If one or both is unavailable then it is instead possible to generate Python scripts which can be processed to product plots at a later date. (This provides a means to customize the plot format, if desired.)

If the [seaborn](#) statistical library is available, CppTransport can use it to style its plots.

- If the [Graphviz](#) tools are available, the HTML report generator will produce a dependency diagram showing how each product generated by an output task depends on content produced by earlier integration and post-processing tasks.

2.2 Downloading the CppTransport platform

The CppTransport sources can be downloaded from various locations:

- Citeable archives tagged with a unique DOI and containing the source code are deposited at the CERN/OpenAIRE Zenodo repository

<https://zenodo.org/record/61237>

- The same tar archives can be downloaded from <http://transportmethod.com>, or from CppTransport’s GitHub homepage:

<https://github.com/ds283/CppTransport/releases>

- If you wish to install a pre-release version of CppTransport, or contribute to its development, you can fork or clone the git repository from GitHub.

Reporting issues.—Bug reports, feature requests or other issues are best reported using the issue tracker on the GitHub page:

<https://github.com/ds283/CppTransport/issues>

2.3 Building the translator and installing the runtime system

This section describes how to install CppTransport, with explicit summaries for handling dependencies in a number of common cases—OS X with MacPorts or Homebrew, and Ubuntu. Users with experience building and installing software may wish to skip directly to §2.4 which gives instructions for building the CppTransport once all dependencies have been installed.

2.3.1 Installing dependencies on OS X

As explained above, to build on OS X it is usually convenient to use the MacPorts or Homebrew packaging systems to simplify installation of its dependencies. Whichever package manager is chosen, the first step is to install Xcode and its associated command-line tools.

1. Download Xcode from the App Store. It is a large download (roughly ~ 6 Gb) so this may take a while.
2. Install the command-line tools associated with Xcode by opening the Terminal application and typing:

```
1 xcode-select --install
```

3. Agree to the Xcode license by typing:

```
1 sudo xcodebuild -license
```

You will need to page to the end of the license or chose `q` to quit, followed by typing `agree` to confirm that you accept the license.

Using MacPorts.—To install CppTransport’s dependencies using MacPorts:

1. Install the MacPorts system from <http://www.macports.org>. Installers are available for each recent release of OS X.
2. Once MacPorts is installed, open a new Terminal. (MacPorts makes some changes to your configuration files in order to make its packages available. These changes are only picked up when you open a new Terminal.)

The dependencies for CppTransport can be installed simultaneously by typing

```
1 sudo port install cmake openmpi boost +openmpi ginac openssl
```

(Note that the combination `boost +openmpi` is a single item and instructs MacPorts to install the Boost libraries using OpenMPI as the MPI implementation.) Each of these packages has further dependencies which MacPorts will download and install automatically. This process can take some time.

If you want to use Python to produce plots and Graphviz for dependency diagrams then this can be followed with

```
1 sudo port install py-matplotlib py-seaborn graphviz
```

Alternatively you can combine all these packages together in a single `sudo port install` instruction.

3. When all packages have installed, issue the command

```
1 sudo port select --set mpi openmpi-mp-fortran
```

This selects OpenMPI as the default MPI implementation, which will enable CppTransport to find its libraries while it is being built.

Using Homebrew.—The procedure is similar for Homebrew.

- Install Homebrew by following the instructions at <http://brew.sh>.
- To install the major CppTransport dependencies, execute

```
1 brew install cmake openmpi ginac openssl
2 brew install boost --c++11 --with-mpi --without-single
```

- Although Homebrew includes Python and Graphviz it does not include Matplotlib, which must be installed separately. First install Python and Graphviz:

```
1 brew install python graphviz
```

We will also want two further dependencies:

```
1 brew install pkg-config pip
```

It is now possible to install Matplotlib and seaborn:

```
1 pip2 install matplotlib seaborn
```

2.3.2 Installing dependencies on Ubuntu 16.04

Most Linux distributions will include packages for all CppTransport dependencies. For illustration we describe the process for Ubuntu 16.04, but the process will be nearly unchanged for any Debian-based distribution.

From a terminal, issue the command:

```
1 sudo apt-get install libsqlite3-dev libboost-all-dev libginac-dev libopenmpi-dev libssl-dev cmake
  ↪ python-matplotlib python-seaborn graphviz git texlive texlive-latex-extra
  ↪ texlive-fonts-recommended
```

This will download and install all required packages and their dependencies. Depending what is already available on your machine, this may be a sizeable download and could take some time. The large `texlive` dependencies are needed only if you plan to use L^AT_EX typesetting with Matplotlib.

Ubuntu provides a tool called `ubuntu-make` which can conveniently [install development platforms](#) and their dependencies. Although alternatives exist, you may wish to investigate the [CLion](#) and [DataGrip](#) platforms which are available through `ubuntu-make`. These are commercial products, but free licenses are available to researchers with an academic email address. In particular, [DataGrip](#) is a good candidate for a tool to manage or interrogate the SQL databases that CppTransport produces (see §4.4.2).

2.4 Building the translator

Once all dependencies are installed it is possible to build CppTransport. Assuming you have downloaded the source code from [zenodo.org](#), [transportmethod.com](#) or as a specific release from [GitHub](#), it will be packaged as a `.tar.gz` archive containing the source tree. Place this archive in a suitable directory, then unpack the archive by typing

```
1 tar xvf CppTransport_2016_03.tar.gz
```

The name of the archive may be different if you are using a more recent version. The CppTransport source code will be unpacked into a directory with the name `CppTransport`. The build process proceeds by entering this directory, creating a *new* directory called `build` that will hold temporary files, and then configuring CMake to use your preferred compiler and install to your preferred location.

CppTransport can be installed *system-wide*, making it available to all users on a machine. Alternatively it can be installed locally, just for a single user. For example, if installing system wide we might choose to locate it in `/usr/local`. This usually requires administrator privileges. Single-user installation would usually locate CppTransport within the user's home directory and does not require administrator privileges. This may be the only option if you are building on a managed system such as a cluster.

In what follows we shall assume that installation is happening locally, but the changes required for system-wide installation are minimal. First, enter the CppTransport directory and create a new directory for temporary files:

```
1 cd CppTransport
2 mkdir build
3 cd build
```

The next step is to configure CMake. If you are building with the default compiler you can enter


```
1 cmake .. -DCMAKE_BUILD_TYPE=Release -DCMAKE_INSTALL_PREFIX=~/.cpptransport-packages
```

This instructs CMake to build using a release configuration (some debugging code is suppressed) and install to the directory `~/.cpptransport-packages`. The precise name of this directory is arbitrary and can be freely changed, although it is wise to avoid the names `~/.cpptransport` and `~/.cpptransport_runtime` which CppTransport expects to be associated with configuration files. (See the discussion on p.16 below.) If you are installing system-wide the install prefix should be set using `-DCMAKE_INSTALL_PREFIX=/usr/local` or similar.

If you wish to build with a different compiler then CMake will require further information. For example, if the Intel compiler is available on your `PATH` and you wish to build with it, you should use

```
1 cmake .. -DCMAKE_BUILD_TYPE=Release -DCMAKE_INSTALL_PREFIX=~/.cpptransport-packages
  ↪ -DCMAKE_C_COMPILER=icc -DCMAKE_CXX_COMPILER=icpc
```

More generally, you should pass the location of the C compiler as the value of `CMAKE_C_COMPILER` and the location of the C++ compiler as the value of `CMAKE_CXX_COMPILER`.

If configuration is successful, build the translator and then install:

```
1 make CppTransport -j4
2 make install
```

Adjust the argument `-j4` to correspond to the number of cores available on your machine; for example, on a dual-core machine you should use `-j2` and on a quad-core machine with hyperthreading you could use `-j8`. If you don't wish to use parallelized builds then it is possible to omit the `-j` argument altogether, although the process may take substantially longer.

2.5 Configuring your environment

PATH variable.—CppTransport is now installed, but is not yet usable. The install procedure writes a large number of files and resources into directories under the installation prefix specified in `CMAKE_INSTALL_PREFIX`; see Fig. 2. One of these files is the translator, called CppTransport, which is installed under `bin`. The operating system needs to know where to find this when we ask it to process a model file, and this means adding its parent directory to the `PATH` variable. We also have to inform CppTransport where its supporting files have been installed; for example, the translator requires access to its templates, and the runtime environment requires access to various assets that are used when writing HTML reports.

The first step is to add the `bin` directory to your path. Typically this would be set in a configuration script such as `.profile`.⁵ You may find that this file already contains a line of the form

```
1 export PATH=/opt/local/bin:/opt/local/sbin:$PATH
```

⁵There are several possible locations where `PATH` can be set, but `.profile` is a good choice because it will typically be read for non-interactive shells. This can be important if you will be running CppTransport via MPI in a cluster environment.

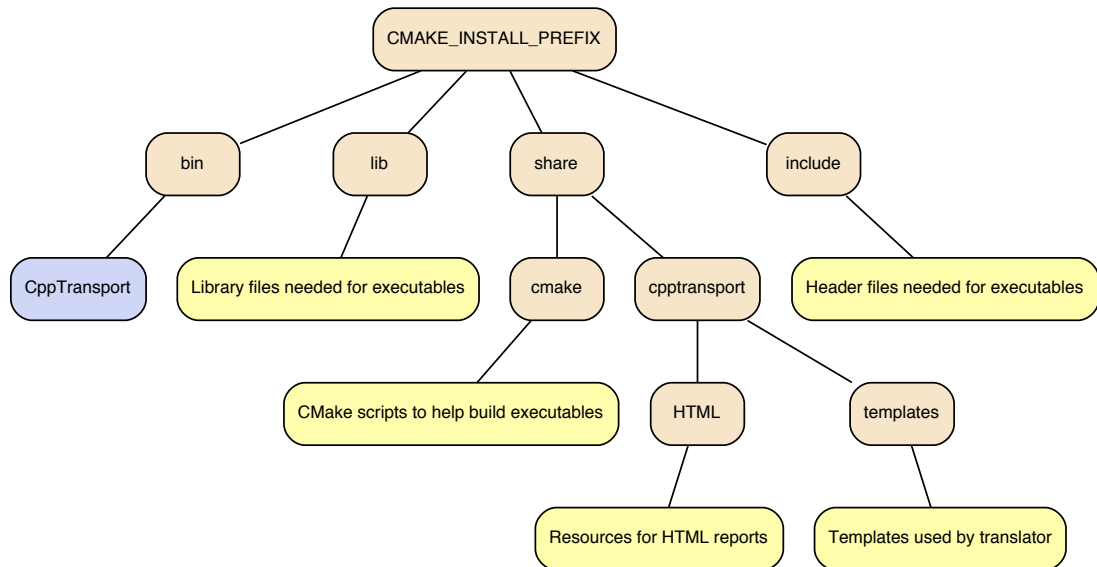


Figure 2. Directory structure created by CppTransport installation process.

although the precise list of colon-separated paths may be different. If not, or there was no existing `.profile` script, add a new entry that points to the `bin` directory under your installation prefix. For example, for a user named `ds283` the resulting line might be

```
1 export PATH=/Users/ds283/.cppttransport-packages/bin:$PATH
```

Ensure that you *add* to the list of colon-separated paths rather than replacing any existing ones, or you may find that you lose access to some of your installed software.

CppTransport resources.—At this stage it should be possible to invoke the CppTransport translator simply by typing `CppTransport` at the command line. and it is worth opening a new terminal (causing your `~/.profile` script to be read) to check that this happens.

```
1 CppTransport --version
```

The translator should respond by printing information about the installed version, such as

```
CppTransport 2016.3 (c) University of Sussex 2016
```

If this has worked successfully then nothing else need to be done to translate model files or build them into executables. The only step that is still required is to inform the runtime system where it can find the files installed under `share`. There are two ways to do this:

- **Use the `CPPTRANSPORT_PATH` environment variable.** CppTransport will search a list of filesystem locations when looking for files. One option is to supply this information as a colon-separated list in the environment variable `CPPTRANSPORT_PATH`, which functions very like the variable `PATH` used above to inform the shell where it should search for executable files.

If set, `CPPTRANSPORT_PATH` should point to the subdirectory `share/cppttransport` of the installation prefix. For example, your `~/.profile` could include a line such as

```
1 export CPPTRANSPORT_PATH=~/.cpptransport-packages/share/cpptransport
```

The `CPPTRANSPORT_PATH` variable is used by both the translator and the runtime library.

- **Use configuration files.** Alternatively, options may be supplied to CppTransport using configuration files in the top level of your home directory. The translator will look for a configuration file named `~/.cpptransport`, and the runtime environment will look for a file named `~/.cpptransport_runtime`. The use of separate files enables different options to be passed to each component.

This method allows you to avoid adding extra material to your `~/.profile` script (or related files), if that is desirable. To use configuration files for this purpose, create a `~/.cpptransport` file containing a the line such as

```
1 include = /Users/ds283/.cpptransport-packages/share/cpptransport
```

where the path on the right-hand side should be adjusted to have the correct prefix and home directory. Notice that although is the same path that would appear in `CPPTRANSPORT_PATH`, the symbol `~` cannot be used to represent the path to the home directory.

The runtime system requires a separate configuration file called `.cpptransport_runtime` which should include the same line:

```
1 include = /Users/ds283/.cpptransport-packages/share/cpptransport
```

Using Python to produce plots.—Provided the Python interpreter is available on your `PATH` it will be automatically detected. CppTransport will also detect whether Matplotlib is available. Therefore it is not necessary to adjust any settings in order to use these tools.

By default CppTransport will produce plots in Matplotlib’s own default style. This was designed to mimic the appearance of MatLab and is not ideal for publication-quality results. If the installed version of Matplotlib is sufficiently recent to support [style sheets](#), or if the `seaborn` package is available, then CppTransport can use these features to produce more attractive output. These features are enabled using the `plot-style` option. This can be provided on the command line (see §8.2), but it is usually more convenient to include it in the `~/.cpptransport_runtime` configuration file. This file should include a line such as

```
1 plot-style = seaborn
```

Currently, the available styles are `ggplot`, `ticks` (corresponding to the Matplotlib style sheets with the same name; for example, see [here](#)) and `seaborn`. If you wish to use a different style it is possible to generate Python scripts from an output task and insert any required customization by hand.

If you are running CppTransport via SSH or a similar remote login, you may need to force Matplotlib to use a noninteractive backend. By default CppTransport will use whatever backend has already been configured; for more details, [see the Matplotlib documentation](#). If Matplotlib has been configured to use an interactive backend this will usually fail for jobs started via remote login. To fix this you should force CppTransport to use a noninteractive backend using the `--mpl-backend` option. The allowed backends are `Agg`, `Cairo`, `PDF`

and `MacOSX`. The Cairo renderer sometimes has problems with L^AT_EX-formatted text. The `Agg` backend is a good choice unless you know you need something different. To set this permanently, add line line

```
1  mpl-backend = Agg
```

to your `~/ .cpptransport_runtime` file.

Using Graphviz.—As for Python, CppTransport will automatically detect the Graphviz tools, provided they are available on your `PATH`.

3 The translator: generating custom code for a specific model

The first step in using CppTransport to perform practical calculations is to generate a *model description file*. As explained above, this describes details of the inflationary model such as its field content and Lagrangian. It is used by the translator to generate specialized code capable of computing the required initial conditions and transport equations. This code is constructed from a supplied template by applying well-defined replacement rules. The template can be modified if required, but in practice this is not normally necessary.

Warning

Will CppTransport work for my model?—Before using CppTransport to study a model, you should carefully evaluate whether it satisfies the criteria for applicability of the underlying numerical scheme. For more details see the accompanying technical paper [44]. The key considerations are:

- **Is it possible to find an initial time at which the slow-roll conditions approximately apply?** CppTransport needs initial estimates of the two- and three-point correlation functions, which are obtained from analytic methods that use the slow-roll approximation.

Although the slow-roll conditions normally do not have to be strongly satisfied at the initial time, they should be *approximately* satisfied in order that the analytic estimates fall within the basin of attraction of the true numerical solution. Usually the initial conditions will safely relax to this true value, although there is no guarantee that this will always happen.

- **Does the tree approximation apply?** CppTransport implements a numerical scheme that computes tree-level estimates of each correlation function. For many models this is safe, but you should exercise caution if:
 - loop corrections are already important for S-matrix processes such as scattering or decays
 - copious particle production could allow significant contributions to the curvature perturbation ζ from multiparticle production channels. Multiparticle channels such as $n \rightarrow 1$ decay for $n \geq 2$ make loop-level contributions to expectation values, even if the $n \rightarrow 1$ process itself is tree-level when considered as an S-matrix element. For more details, see §3.1 of Ref. [44].

- production of finite-wavenumber modes can significantly drain energy from the zero-mode, as in warm inflation or trapped inflation.

The model description file consists of a number of *blocks* that declare properties and attributes for the model. They generally take the form

```
block-name tag { attribute-list }
```

Here, *block-name* is a keyword indicating what kind of attributes are being declared; *tag* is a label used to identify the block; and *attribute-list* is a list of assignments in the form

```
property = value;
```

Breaking the model description into files.—If desired, it is possible to spread the model description over several files by using the directive `#include "string"`. The effect is as if the contents of the file whose name matches `string` had been included at the same point. The included file can itself contain further `#include` directives.

3.1 Adding model metadata

Blocks can come in any order, but it is generally preferable to place the `model` block at or near the top of the file because it contains a range of useful summary information. Most of the fields are optional, but if provided they are embedded within the custom C++ output and subsequently attached to any data products that it is used to generate. By specifying this data we reduce the risk of ‘orphaned’ code or data that cannot be traced back to a specific combination of model, parameters and initial conditions.

The attributes available within the `model` block are:

- The tag: this is used to construct the names of the C++ classes build by the translator, and also the names of the output files it generates. For this reason it should be fairly short and obey the rules for constructing valid C++ identifiers and filenames.,
- `name = "string";`
Sets the model’s textual name to `string`. The textual name is generally used only when producing reports; automatically-generated code normally refers to the model using the tag associated with the block.
- `description = "string";`
Adds a short description of the model. This should briefly identify its origin and major features.
- `citeguide = "string";`
Give short guidance about how to cite this model and its description file.
- `license = "string";`
If you intend to make your description file publicly available (eg. on the arXiv or via a data repository service such as zenodo.org), you may wish to explicitly set a license that allows re-use such as the [Creative Commons Attribution license](https://creativecommons.org/licenses/by/4.0/). Some funding agencies may express a preference (or even specific requirements) for the licensing of research outputs.

- `revision = integer;`
A model description may evolve through multiple iterations during its lifetime. Where significant changes occur it can be helpful to indicate this unambiguously by changing the model’s textual name and the tag used to identify it in generated C++. However, for minor changes it may be less confusing to retain the same identifiers. In these circumstances the `revision` field can be used to distinguish between different versions of the model file.

The runtime system will not allow code generated using an earlier revision of a model description file to handle tasks prepared using a later revision.
- `references = [string, string, ...];`
Attach a comma-separated list of strings that reference publications associated with this model. The strings are free-format and can be used for any suitable purpose. For example, you may wish to identify papers by their arXiv number or by DOI.
- `urls = [string, string, ...];`
Attach a comma-separated list of strings corresponding to URLs associated with this model. These should be internet locations to which an end-user can refer to obtain more details about the model or its implementation.

Example

To illustrate the process of preparing a model file and constructing tasks, in these panels we will work through the steps needed for the model of double quadratic inflation—eventually building up to an analysis of its bispectrum.

This model was introduced by Rigopoulos, Shellard & van Tent [46, 47] and later studied by Vernizzi & Wands [48]. It has been widely used as a test case for numerical methods; see eg. Refs. [49, 50].

CppTransport does not expect any particular naming convention for model description files, and they do not need to have a fixed extension. However, to keep them readily recognizable it may help to apply a uniform extension such as `.model` or `.mdl`. In this case we will write the model description into a file named `dquad.model`. The first step is to construct a suitable `model` block. We use the tag `"dquad"`, and provide links to the original literature. We also assign the model file a specific license by tagging it with the abbreviation “CC BY”, which indicates the Creative Commons Attribution License.

```

1  model "dquad"
2  {
3      name           = "Double quadratic inflation";
4      description    = "A two-field model with quadratic potentials";
5      citeguide      = "Example from the CppTransport user guide";
6      license        = "CC BY";
7      revision       = 1;
8
9      references     = [ "astro-ph/0504508",
10                       "astro-ph/0511041",
11                       "astro-ph/0603799",
12                       "arXiv:160x.yyyy" ];
13     urls           = [ "http://transportmethod.com" ];
14 };

```

3.2 Specifying a template

The translator produces customized C++ output by reading the model description file, using it to construct all the information needed for concrete calculations, and then writing this information into a *template*. We will examine this process in more detail in §3.7. CppTransport allows arbitrary templates to be used, although there will not normally be any need to modify the supplied examples. The purpose of the `model` block is to tell CppTransport which templates are intended for use. It does not have a tag.

To use the standard templates, the `templates` block should read:

```

1  templates
2  {
3      core           = "canonical_core";
4      implementation = "canonical_mpi";
5  };

```

Notice that two templates are required. The *core* template writes an output file called `tag_core.h` and defines a C++ class called `tag_core`, where `tag` is the tag used to declare the `model` block. This class provides common services such as computation of initial conditions and mass matrices, which are the same no matter how we choose to solve the equations of motion for each correlation function. The *implementation* class defines a C++ class that integrates these equations.

In principle CppTransport can support many different implementations. For example, these could use different resources to carry out the calculation, perhaps by splitting the work across a range of CPUs and offload processors such as GPUs or Xeon Phis. Currently only an MPI-based CPU integrator is supplied because testing has shown that—for the specific system of differential equations that CppTransport needs to solve—it is not straightforward to extract good performance from GPUs. This difficulty is partially driven by memory requirements, and may change in future. The CPU integrator is supplied as a template called `canonical_mpi.h` and writes an output file called `tag_mpi.h`. It defines a C++ class called `tag_mpi`.

3.3 Choosing a stepper

The translator customizes the integration template to use a stepper drawn from the Boost.odeint [collection](#). Not all the steppers provided by odeint are available, and the selection may expand

in future. Currently, the supported steppers are:

- **runge_kutta_dopri5**. This is a 4th/5th-order Dormand–Prince solver, and a good general purpose stepper. It is capable of efficiently interpolating the solution between sample points, meaning that the step-size can often be kept large even when high accuracy is required. This gives the method good overall performance. It should be regarded as the default unless the model requires special treatment.
- **runge_kutta_fehl78**. This is a 7th/8th order Fehlberg solver. It is higher-order than the Dormand–Prince algorithm, but cannot interpolate the solution between sample points and therefore sometimes struggles to control its step-size. Nevertheless, it remains a useful alternative.
- **bulirsch_stoer_dense_out**. This is a Bulirsch–Stoer algorithm that adapts both its step-size and the order of the method, currently up to 8th order. It can interpolate the solution, enabling the same good control of step-size exhibited by the Dormand–Prince algorithm. It is typically slower than the other algorithms but is a good choice where high precision is required. It may be the only practical choice if the solution exhibits sharp features, which the adaptive order control can handle quite effectively.

No matter which stepper is selected, it is a good idea to check that features in a solution are stable to changes in the stepper and sample mesh.

Because the background equations seldom require a stepper with advanced capabilities it is possible to specify separate steppers for the background and perturbations. At present this has limited utility because background integrations usually constitute a negligible proportion of the runtime, but it may have more impact in future.

The background stepper is specified with a `background` block, and the stepper for perturbations is specified with a `perturbations` block. Each block accepts the same attributes, and neither has a tag.

- `stepper = "string";`
Sets the stepper for this block to be one of the supported steppers listed above.
- `stepsize = number;`
Sets the initial step-size. All steppers supported by CppTransport are adaptive and will adjust their step-size depending on the structure of the solution, but an initial estimate is needed. The step-size is measured in e-folds. Typically values in the range 10^{-12} to 10^{-15} are reasonable. The stepsize will rapidly be adjusted upwards if the solution makes this practicable.
- `abserr = number;`
Sets the absolute tolerance for the stepper.
- `relerr = number;`
Sets the relative tolerance for the stepper.

Suitable values for the tolerances are typically in the range 10^{-8} to 10^{-12} , although in some cases they need to be smaller. A reasonable default choice is 10^{-8} , followed by reduction to 10^{-10} or 10^{-12} if the stepper fails to keep the solution under control.

Example

Nothing special is needed for the double-quadratic model, so we can use the default `runge_kutta_dopri5` solver and conventional values for the step-size and tolerances. In addition we are using the standard templates, so we should add the following lines to the description:

```
1 templates
2 {
3     core          = "canonical_core";
4     implementation = "canonical_mpi";
5 };
6
7 background
8 {
9     stepper = "runge_kutta_dopri5";
10    stepsize = 1E-12;
11    abserr  = 1E-12;
12    relerr  = 1E-12;
13 };
14
15 perturbations
16 {
17     stepper = "runge_kutta_dopri5";
18     stepsize = 1E-12;
19     abserr  = 1E-12;
20     relerr  = 1E-12;
21 };
```

3.4 Adding author metadata

The authors of the model description file can be identified by including one or more `author` blocks. In principle these are intended to identify the authors of the *model description* rather than to assign credit for the original model, which can be done via the `references` attribute of the `model` block.

The tag for each block should be a string giving the author's textual name. The available attributes are:

- `email = "string";`
Attaches an email address for this author. Only one address is allowed per author. If multiple email attributes are given then the translator will issue a warning.
- `institute = "string";`
Attach an institutional affiliation. As with email addresses, only one affiliation is allowed per author.

Example

A suitable author block for our example file might be:

```

1 author "David Seery"
2 {
3     institute = "Astronomy Centre, University of Sussex";
4     email     = "D.Seery@sussex.ac.uk";
5 };

```

3.5 Specifying field content and Lagrangian parameters

The final step is to specify the Lagrangian of the model. Because CppTransport is currently restricted to models with canonical kinetic terms it is only necessary to specify the potential. Before doing so, we must enumerate the fields used by the model and any parameters appearing in the Lagrangian. This is done by giving a `field` block for each field, and a `parameter` block for each parameter. The tag for each block is a symbolic name that can be used to refer to the corresponding quantity in the potential. Currently, only one attribute is available which is used to give a \LaTeX name for the quantity:

- `latex = "string";`
Set the \LaTeX name of the quantity to be `string`. The \LaTeX name is available for use when generating derived products such as plots.

Example

In the double-quadratic inflation there are two fields, conventionally ϕ and χ , and the potential is

$$V(\phi, \chi) = \frac{1}{2}M_\phi^2\phi^2 + \frac{1}{2}M_\chi^2\chi^2. \quad (3.1)$$

This means there are two parameters, M_ϕ and M_χ . To declare all of these objects we would write

```

1 field phi
2 {
3     latex = "\phi";
4 };
5
6 field chi
7 {
8     latex = "\chi";
9 };
10
11 parameter Mphi
12 {
13     latex = "M_\phi";
14 };
15
16 parameter Mchi
17 {
18     latex = "M_\chi";
19 };

```

3.6 Specifying the Lagrangian

Once all fields and parameters have been declared we can use them to give an expression for the potential. The syntax for this is `potential = expression;` where `expression` is a mathe-

function	meaning
<code>abs(x)</code>	absolute value $ x $
<code>sqrt(x)</code>	square root \sqrt{x}
<code>sin(x)</code>	sine $\sin x$
<code>cos(x)</code>	cosine $\cos x$
<code>tan(x)</code>	tangent $\tan x$
<code>asin(x)</code>	inverse sine $\sin^{-1} x$
<code>acos(x)</code>	inverse cosine $\cos^{-1} x$
<code>atan(x)</code>	inverse tangent $\tan^{-1} x$
<code>atan2(y,x)</code>	inverse tangent $\tan^{-1} y/x$ using signs of x, y to determine quadrant
<code>sinh(x)</code>	hyperbolic sine $\sinh x$
<code>cosh(x)</code>	hyperbolic cosine $\cosh x$
<code>tanh(x)</code>	hyperbolic tangent $\tanh x$
<code>asinh(x)</code>	inverse hyperbolic sine $\sinh^{-1} x$
<code>acosh(x)</code>	inverse hyperbolic cosine $\cosh^{-1} x$
<code>atanh(x)</code>	inverse hyperbolic tangent $\tanh^{-1} x$
<code>log(x)</code>	natural logarithm $\ln x$
<code>pow(x, y)</code>	exponentiation x^y

Table 1. Mathematical functions understood by CppTransport

mathematical expression written using the same kind of syntax one would employ in *Mathematica* or *Maple*. CppTransport understands the standard mathematical operators, including `+` for addition, `-` for subtraction, `*` for multiplication, `/` for division and `^` for exponentiation. Nested brackets `(...)` can be used to indicate precedence. It also understands the mathematical functions listed in Table 1.

In simple cases it is easy to specify the potential in just one line. For example, in single-field ϕ^2 inflation we could write

```
1 potential = m^2 * phi^2 / 2;
```

Fields are assumed to have dimension $[M]$, and the pre-defined symbol `M_P` is available to represent the Planck mass.

In more complex cases, single-line expressions become difficult to read or debug and it is preferable to break the potential down into subexpressions. CppTransport provides a `subexpr` block for this purpose. Its tag is the symbol that will be used to refer to the subexpression, and the block accepts two attributes:

- `latex = "string";`
Specifies a L^AT_EX symbol associated with this subexpression.

- `value = expression;`
Defines the symbolic expression associated with this quantity.

For example, consider the potential studied by Gao, Langlois & Mizuno [51],

$$V(\phi, \chi) = \frac{1}{2}M^2[\chi - (\phi - \phi_0) \tan \Xi]^2 \cos^2 \frac{\Delta\theta}{2} + \frac{1}{2}m_\phi^2\phi^2, \quad (3.2)$$

where Ξ is defined by

$$\Xi \equiv \frac{\Delta\theta}{\pi} \tan^{-1} \frac{s(\phi - \phi_0)}{M_P^2}. \quad (3.3)$$

This potential is designed to contain an inflationary valley with a turn. The quantities M and m_ϕ are mass scales, and ϕ_0 , $\Delta\theta$ and s are constants that parametrize the turn. Assuming we have defined suitable fields `phi`, `chi` and parameters `M`, `mphi`, `phi0`, `Delta` and `s`, the potential can be broken down into subexpressions:

```

1  subexpr Xi
2  {
3    latex = "\Xi";
4    value = (Delta/pi) * atan(s*(phi-phi0) / M_P^2);
5  };
6
7  subexpr V1
8  {
9    latex = "V_1";
10   value = (1/2) * M^2 * (chi - (phi-phi0)*tan(Xi))^2 * cos(Delta/2)^2;
11 };
12
13 subexpr V2
14 {
15   latex = "V_2";
16   value = (1/2) * mphi^2 * phi^2;
17 };
18
19 potential = V1 + V2;
```

Example

The potential for double-quadratic inflation is simple. Given the fields and parameter definitions described above it can be written in one line:

```
1 potential = Mphi^2 * phi^2 / 2 + Mchi^2 * chi^2 / 2;
```

3.7 Running the translator and producing output

Once the model description is complete, the translator is run to produce C++ classes that implement the transport equations for it. Provided your environment has been set up as described in §2.5 it should be possible to invoke the translator simply by typing `CppTransport` at the shell prompt.

The translator accepts a number of arguments. Some of these perform simple house-keeping functions:

- `--help`
Display brief usage information and a list of all available options

- **--version**
Show information about the version of CppTransport being used.
- **--license**
Display licensing information.
- **--no-colour** or **--no-color**
Do not produce colourized output. CppTransport will normally detect the type of terminal in which it is running and adjust its output formatting appropriately. Where colour is available, it is used to add clarity. However, if you are redirecting its output to a file (or if this happens automatically as part of a batch environment), you may wish to suppress this behaviour.
- **--verbose**, or abbreviate to **-v**
Enable verbose output, giving more information about the different phases of translation and some statistics about the process.

Others affect the files read or written by the translator:

- **--include**, or abbreviate to **-I**
Should be followed by a path to be added to the list of paths searched when looking for template files. For example, if extra templates have been written (or installed in a different location), this argument can be used to enable CppTransport to find them. The templates should be stored in a directory named `templates` under this path.
- **--no-search-env**
Do not use the environment variable `CPPTRANSPORT_PATH` to determine a list of search paths; use only paths specified by **--include** on the command line.
- **--core-output**
Followed by a path that specifies the file to which the customized *core template* should be written. By default the name `tag_core.h` is used, where `tag` is the tag used to declare the `model` block. In most cases this default will be suitable, so it is not necessary to specify a filename explicitly.
- **--implementation-output**
Followed by a path that specifies the file to which the customized *implementation template* should be written. By default the name `tag_implementation.h` is used, where `tag` is the tag used to declare the `model` block and `implementation` is the name of the integration implementation; in the current version this is always `mpi`. In most cases this default will be suitable, so it is not necessary to specify a filename explicitly.

A final set of options influence the C++ code generated by the translator:

- **--no-cse**
Disable *common sub-expression elimination*, described in more detail in §3.8 below.
- **--annotate**
Annotate the generated code with comments, including comments to indicate which template line corresponds to each output line. This option can be useful for debugging, but often generates large files.

- **--unroll-policy**
Followed by an integer corresponding to the maximum allowed size of an *unrolled index set*, described in more detail in §3.8.
- **--fast**
Unroll all index sets, regardless of size.

These options may also be specified in the `~/ .cpptransport` configuration file discussed on p.16. Each option should be placed on a new line, without the leading `--`. Options such as `--include` that accept an argument should be written in the format `option = argument`, such as `include = /usr/local/share/cpptransport` as described above. If an option appears both in the configuration file and on the command line, then values specified on the command line are preferred.

Example

For double-quadratic inflation no special options are required (although see the discussion of `--fast` in §3.8 below, which can be used to improve the execution time for this model). To print status messages during the different phases of translation we can run the translator with the `--verbose` or `-v` switch to produce verbose output. This gives:

```
$ CppTransport -v dquad.model
CppTransport: translating '../templates/canonical_core.h' into 'dquad_core.h'
CppTransport: translation finished with 1216 macro replacements
CppTransport: macro replacement took 0.172s, of which time spent tokenizing 0.00881s (symbolic
↳ computation 0.0223s, common sub-expression elimination 0.087s)
CppTransport: translating '../templates/canonical_mpi.h' into 'dquad_mpi.h'
CppTransport: translation finished with 8102 macro replacements
CppTransport: macro replacement took 0.169s, of which time spent tokenizing 0.00547s (symbolic
↳ computation 0.0179s, common sub-expression elimination 0.0919s)
CppTransport: 153 expression cache hits, 415 misses (time spent performing queries 0.0116s)
CppTransport: processed 1 model in time 0.391s
```

CppTransport gives information about each file it translates. Here, the files being translated are the core template `canonical_core` which becomes `dquad_core.h`, and the implementation template `canonical_mpi` which becomes `dquad_mpi.h`. Recall that the stem `dquad` used to construct these filenames is taken from the tag provided to the model block in §3.1.

In the subsequent messages, CppTransport informs us of the number of tokens (‘macros’) replaced while customizing each file, and also the time spent performing each step. Sometimes common sub-expression elimination becomes very time-consuming; in this case, see the discussion in §3.8.

3.8 Using the code generation options

As explained above, the translator’s task is to produce customized output. It does this by rewriting the template files according to well-defined rules.

In order to perform this rewriting the translator recognizes a large number of *tokens*, of the form `$NAME`, `$CITEGUIDE`, `$DESCRIPTION` (and so on), which are replaced with the corresponding data from the model description file. There are also tokens such as `$HUBBLE_SQ` and `$EPSILON`

which are replaced with symbolic expressions computed from the Lagrangian of the model—here, these would be expressions to compute the square of the Hubble rate H^2 and the slow-roll parameter $\epsilon = -\dot{H}/H^2$, respectively.

Unrolling index sets.—In addition to these simple rewriting rules, the translator must be able to generate code that implements the transport equations for the two- and three-point functions. Writing these correlation functions as

$$\begin{aligned}\langle \delta\phi^\alpha(\mathbf{k}_1)\delta\phi^\beta(\mathbf{k}_2) \rangle_t &= (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2) \Sigma^{\alpha\beta} \\ \langle \delta\phi^\alpha(\mathbf{k}_1)\delta\phi^\beta(\mathbf{k}_2)\delta\phi^\gamma(\mathbf{k}_3) \rangle_t &= (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) \alpha^{\alpha\beta\gamma},\end{aligned}\tag{3.4}$$

their evolution equations become

$$\begin{aligned}\frac{d\Sigma^{\alpha\beta}}{dN} &= u^\alpha{}_\gamma \Sigma^{\gamma\beta} + u^\beta{}_\gamma \Sigma^{\alpha\gamma} \\ \frac{d\alpha^{\alpha\beta\gamma}}{dN} &= u^\alpha{}_\delta \alpha^{\delta\beta\gamma} + u^\alpha{}_{\delta\epsilon} \Sigma^{\delta\beta} \Sigma^{\epsilon\gamma} + \text{cyclic},\end{aligned}\tag{3.5}$$

where $dN = H dt$ represents the number of e-folds which elapse in a cosmic time interval dt . Here, $u^\alpha{}_\beta$ and $u^\alpha{}_{\beta\gamma}$ are coefficient matrices calculated internally by the translator and depending on the wavenumbers $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3$. These matrices are represented using further tokens such as `$U2_TENSOR[AB]` (corresponding to $u^\alpha{}_\beta$) and `$U3_TENSOR[ABC]` (corresponding to $u^\alpha{}_{\beta\gamma}$). The labels `[AB]` and `[ABC]` represent the associated indices. The translator understands enough of the Einstein summation convention to represent (for example) the transport equation for the two-point function as

```
1 dSigma[$A][$B] $= $U2_TENSOR[AC] * Sigma[$C][$B];
2 dSigma[$A][$B] $+= $U2_TENSOR[BC] * Sigma[$A][$C];
```

It has been assumed that the two-point function $\Sigma^{\alpha\beta}$ is encoded in an array-like object `Sigma[] []` and the derivative is to be written into a separate array-like object `dSigma[] []`. In particular, given these expressions the translator understands that the free indices `[A]` and `[B]` label independent components of the overall matrix equation, and that the repeated index `[C]` is to be summed over. The transport equation for the three-point function can be represented similarly.

During translation these compact expressions must be unpacked into valid C++ that performs the required calculations. There are N^2 independent equations for the two-point function, each of which entails a sum over one dummy index. Therefore the overall size for this set of equations scales as $O(N^3)$. For the three-point function there are N^3 independent equations, but now each equation entails a sum over *two* dummy indices. Therefore the overall size scales as $O(N^5)$. After unpacking we incur two types of cost. One is *execution time*: no matter how they are expressed, the amount of work involved in solving these evolution equations will scale roughly like $O(N^3)$ or $O(N^5)$, respectively. The other is *space*: if unpacked in the most literal fashion, by simply writing out each component of Eq. (3.5) sequentially, the size of the generated C++ code will also scale roughly like $O(N^3)$ or $O(N^5)$.

We cannot alter the power law in these scalings, but it is possible to make some limited tradeoffs between the space cost and execution time:

- To obtain the fastest execution time, we can opt for the space-hungry strategy of writing out each equation explicitly. CppTransport describes the indices being unpacked as an *index set*, and refers to the process of writing them out sequentially as *unrolling*.⁶

Unrolling allows the C++ compiler to generate simple linear code that performs all the required computations without branches or jumps, which would be required by loops and may incur performance penalties. Also, because this strategy is completely explicit it maximizes the compiler’s opportunities to optimize away redundant calculations.

The downside is that generated C++ files become very large even for moderate N . If we require the three-point function then the dominant scaling comes from terms of the form $u^{\alpha}_{\delta\epsilon}\Sigma^{\delta\beta}\Sigma^{\epsilon\gamma}$. We have been estimating the number of terms in each sum as $\sim N$, but it is usually $2N$ because we must account both for the fields and their canonical momenta. Therefore, assuming the dominant terms generate $\sim (2N)^5$ lines and supposing each of these lines to average ~ 50 characters, it follows that even $N = 20$ will generate an implementation file of size ~ 10 Gb. Such large files require a prohibitively large amount of time and memory to compile. This places a practical upper limit on the maximum size of a C++ file. On typical hardware this limit is already much smaller than 1 Gb, making unrolling an unacceptable strategy except when N is rather small.

- Alternatively, the indices can be unpacked into a C++ `for`-loop. For example, the translator might unpack the line `dSigma[$A][$B] $= $U2_TENSOR[AC] * Sigma[$C][$B];` into

```

1  for(int A = 0; A < 2*N; ++A)
2  {
3      for(int B = 0; B < 2*N; ++B)
4          {
5              dSigma[A][B] = 0.0;
6              for(int C = 0; C < 2*N; ++C)
7                  {
8                      dSigma[A][B] += U2_TENSOR[A][C] * Sigma[C][B];
9                  }
10         }
11     }

```

assuming that the array-like object `U2_TENSOR[][]` has been initialized with the components of the tensor u^{α}_{β} .

The loop-based representation is considerably more economical with space, because its storage requirements do not grow with N .⁷ For this reason it is the only viable approach for general N . The disadvantage is that we may forfeit opportunities for optimization.⁸ For example, it sometimes happens that certain components of u^{α}_{β} or $u^{\alpha}_{\beta\gamma}$ are zero, and therefore the corresponding terms in the summation can be omitted. When all expressions are written explicitly it is easy for the compiler to make

⁶The name is borrowed from a very similar [loop optimization technique](#).

⁷To be explicit, it is the storage requirements to express the *algorithm itself* that are under discussion here. The storage requirements for the state variables `Sigma` and `dSigma` always scale with N .

⁸Another disadvantage might come from the extra overhead associated with a loop counter and branch penalties. But the C++ compiler might decide it is worthwhile to optimize the loop by unrolling it anyway, in which case these disadvantages disappear. The disadvantage of masking zeros in u^{α}_{β} or $u^{\alpha}_{\beta\gamma}$ generally cannot be fixed, however, even by a good optimizing compiler.

setting	core	implementation	CPU/configuration	CPU total
<code>--fast</code>	135 kb	649 kb	0.993 s	47 m 17 s
<code>--unroll-policy 1000</code>	145 kb	211 kb	1.60 s	1 h 16 m 20 s
<code>--unroll-policy 0</code>	118 kb	89 kb	2.41 s	1 h 54 m 16 s

Table 2. Comparison of generated code size and execution time for 2856 bispectrum configurations and an axion+quadratic model $V = m^2\phi^2/2 + \Lambda^4(1 - \cos 2\pi f^{-1}\chi)$; see Elliston et al. for a description of the parameters and initial conditions [52]. We use the first set of parameters described in §5.1.2 of that reference. Timings are averages of 3 runs using OS X 10.11.4 and the Apple Clang compiler 7.3.0 on an Ivy Bridge i7-3770 machine. Each CppTransport job used 7 worker processes.

such optimizations. In the loop-based approach the compiler will normally be unable to skip particular iterations of the loop body, and therefore these terms will not be optimized away. The effect of these irrelevant operations can accumulate to a sizeable performance difference over many integrations; see Table 2.

CppTransport attempts to find a compromise between these strategies. It will elect to unroll index sets where the result will not be too large, with the distinction being set by the value assigned to `--unroll-policy`. The default is 1000. Also, the elements of a tensor such as u^α_β are stored in temporary arrays (such as `U2_TENSOR[] []` in the above example) because this is required for large index sets that ‘roll up’ into `for`-loops. Depending on the compiler settings, this use of temporary arrays may inhibit some optimization of redundant arithmetic.

The default unroll policy of 1000 is intended to give reasonable performance for models with modest N , while simultaneously allowing models with large N to be handled. However, we will see shortly that if N is not too large then global unrolling should be preferred. In cases where it is known that the resulting C++ files will be acceptable to the compiler it is possible to force global unrolling using the command-line switch `--fast`. This instructs CppTransport to disregard the unroll policy limit and unroll *all* index sets. In addition, the translator will no longer store the elements of tensors such as u^α_β in a temporary array, but instead cache them in `const` local variables. This gives the compiler the best chance of removing unnecessary operations.

Table 2 shows a comparison of execution times for a particular $N = 2$ model with `--fast` and unrolling limits of 1000 and 0 (forcing roll-up of all index sets). It shows a significant advantage for `--fast`. This is a fairly general phenomenon; testing has shown that models with $N = 2$ or $N = 3$ can often be unrolled effectively, yielding a non-negligible performance improvement.

Common sub-expression elimination.—To keep its generated files as small as possible, CppTransport uses a second strategy called *common sub-expression elimination*. The automated symbolic calculations performed internally by the translator are not automatically simplified, and therefore the results resemble those from Mathematica before application of `Simplify[]` or `FullSimplify[]`. These expressions often share common building blocks, such as the Hubble rate H or the slow-roll parameter ϵ , which CppTransport tries to factor out intelligently.

Even when this has been done there may be further common pieces that can be extracted. For example, after common sub-expression elimination, CppTransport would translate the expression $(A + B + 1)^2 / (A + B)$ into C++ of the form

```
1  const auto temp_1 = A + B;
2  const auto temp_2 = temp_1 + 1.0;
3  const auto temp_3 = temp_2 * temp_2;
4  const auto temp_4 = temp_3 / temp_1;
```

The local variable `temp_4` would be used to represent the value of the expression.

This procedure is generally effective at minimizing the size of the generated code, and therefore making the compiler's job as straightforward as possible. However, the task of finding common sub-expressions is expensive in the same way that Mathematica's `Simplify[]` or `FullSimplify[]` operations can be expensive. For more complex models it is usually the most time-consuming step in the translation process, by a considerable margin. If desired, CppTransport provides the command-line switch `--no-cse` to disable common sub-expression elimination. This will dramatically speed up translation, but leaves the compiler with a harder job because the same task has effectively been transferred to it.

Normally it is advisable to leave common sub-expression elimination enabled unless there is a particular difficulty with performing it for a model.

4 Building and running an integration task

4.1 Coupling a model to the runtime system

Once customized core and header files have been produced, they can be used to perform calculations. This involves connecting the translated files to other components of CppTransport, especially those that are needed to carry out integration tasks. To do so we create a short C++ program; for the double-quadratic example this could be called `dquad.cpp`. A simple implementation takes the form:

```
1  // include implementation header generated by translator
2  #include "dquad_mpi.h"
3
4  int main(int argc, char* argv[])
5  {
6      // set up a task_manager instance to control this process
7      transport::task_manager<> mgr(argc, argv);
8
9      // set up an instance of the double quadratic model
10     std::shared_ptr< transport::dquad_mpi<> > model = mgr.create_model< transport::dquad_mpi<>
    ↪ >();
11
12     // hand off control to the task manager
13     mgr.process();
14
15     return(EXIT_SUCCESS);
16 }
```

This code involves the following steps:

1. First, the implementation header file produced in §2.4 is included using `#include "dquad_mpi.h"`. Nothing else is needed to use the CppTransport runtime system; any necessary library files are automatically included by the implementation header.

2. The only function provided is `main()`. It has three responsibilities:

- (a) **Create a *task manager* instance.** The task manager is a class provided by the runtime system. It is responsible for coordinating what happens during execution. For example: if we are running a parallel computation under MPI, each copy of the executable may be either the master process or a worker. It is the responsibility of the task manager to decide which is correct and behave appropriately.

If it is the master process, the task manager builds a list of work using options specified in the configuration file or on the command line. It scatters these tasks to the workers and coordinates their activity. On the other hand, if it is a worker, the task manager waits for tasks to be issued by the master process and arranges for them to be carried out.

The task manager class is called `task_manager<>`. It shares a common feature with most other CppTransport components: it lives inside the namespace `transport`. This prevents any conflict between symbols defined in user code and those used internally by CppTransport. As for objects defined in any namespace, each CppTransport component should be prefixed by the namespace name and two colons, as in `transport::task_manager`.⁹ The meaning of the brackets `<>` is explained in the *Advanced usage* panel on p.33.

The `task_manager<>` constructor requires the arguments `argc` and `argv` provided to `main()`. It will process these internally. The options understood by the task manager are described in XXX.

- (b) **Create an instance of the implementation class.** Second, we need an instance of the implementation class generated by the translator. As explained in §3.2, this class will be called `tag_mpi` if we use the `canonical_mpi` template. For us this will be `dquad_mpi`. Like `task_manager<>` its name should be followed by angle brackets `<>`.

To create the instance we use the `task_manager<>` method `create_model()`. This is a templated method that requires the name of the instance class to be provided between angle brackets; here, this is `< transport::dquad_mpi >`. The method itself takes no arguments. It returns a *shared smart pointer* to the implementation class instance. The use of `create_model()` is necessary, rather than constructing an instance directly, in order that the CppTransport runtime system is aware of the model and can find it when needed for computations.

Notice that there is no need to explicitly deallocate the pointer `model`. It is deallocated automatically when the smart pointer that manages it is destroyed.

- (c) **Pass control to the task manager.** It is possible to create instances of as many implementation classes as are required. Each one should be constructed using `create_model()`. When all implementation classes have been instantiated, control should be passed to the task manager via its `process()` method.

⁹It is possible pull all symbols defined within the `transport` namespace into the global namespace with the `using` directive, as in for example `using namespace transport;`. However, this practice is not recommended because it risks conflicts between user-space symbols and those belonging to CppTransport itself.

When running as the master, `process()` will distribute tasks to the workers. When running as a worker it will await instructions from the master.

3. Finally, the `process()` method returns when all work has been exhausted. At this point the process should terminate, so we return `EXIT_SUCCESS`.

Most CppTransport executables will contain a `main()` function of almost exactly this form. The general case differs only by providing extra functions to generate tasks and derived products, which will be explained in §4.3 and §7 below.

Advanced usage: Custom integration data types

Like most CppTransport components, `task_manager<>` is a **template class**. This is indicated by the angle brackets `<>` following the object name. A *template* is a class or other object that can be customized by providing a list of data types such as `double` (or other parameters) between the brackets. For CppTransport, the customization takes place in the integration engine, that is capable of integrating the transport equations using any suitable data type. If no type name is given, as in the example above, the integrator will default to `double`.

For almost all users the default choice is suitable, so there is no need to specify a type explicitly. As an alternative, however, it is possible use the single-precision type `float` if the intention is to trade off some accuracy against speed.^a For greater precision it is possible to use `long double`, or even a customized type from a library such as the GNU Multiple Precision Arithmetic Library [GMP](#) or the Class Library for Numbers [CLN](#).^b Using types with higher precision than `double` will increase the computation time (eg. switching to `long double` very roughly doubles the time required), whereas `float` may require less stringent tolerances to prevent to integrator's stepsize becoming very small. Attempting to use types from GMP or CLN will likely require some template specializations to be provided. If so, this will manifest itself as missing symbols reported during the link step.

It is possible to use the same core and implementation classes with different data types, just by changing the type name provided in the template specialization brackets `<...>`. However, the current version of CppTransport does not support mixing different types within the *same* executable because the task manager needs to know which data type is in use, and therefore also requires a template specialization such as `<double>`.

^aAlthough it is often true that `float`s are half as long as `double`s, this is a platform dependent statement. On some platforms there may be no difference between `float` and `double`.

^bThere are some caveats. Although CppTransport can integrate using any required type, for storage it relies on the SQLite engine which expects real numbers to be stored as 64-bit IEEE floating-point numbers. On most platforms this corresponds to a `double`, and in fact the SQLite API is written under this assumption. (For details, see [the SQLite documentation](#). There is only a `sqlite3_bind_double()`, but no comparable method for the other floating-point types.) This means that, no matter what precision was used during integration, CppTransport always stores the results as `double` precision. Using higher precision for intermediate values may still be useful, however, to reduce roundoff error in the integrator.

4.2 Translate and build using a CMake script

It is possible to build CppTransport executables by manually invoking the compiler. However, this is not always convenient because it is necessary to locate the Boost and MPI libraries on which the runtime system depends. The recommended way to build is using a CMake build script. When CppTransport is installed, it provides some CMake tools that are intended to simplify this process.

The CMake build script should be called CMakeLists.txt and placed in the same directory as the main C++ file—for the example of double-quadratic inflation this is the file dquad.mpi described above. A suitable script is:

```
1 CMAKE_MINIMUM_REQUIRED(VERSION 3.0)
2 PROJECT(dquad)
3
4 SET(CMAKE_MODULE_PATH ${CMAKE_MODULE_PATH} "~/cppttransport-packages/share/cmake/")
5
6 SET(CMAKE_CXX_FLAGS_RELEASE "-Ofast -DNDEBUG")
7 SET(CMAKE_C_FLAGS_RELEASE "-Ofast -DNDEBUG")
8
9 FIND_PACKAGE(CppTransport REQUIRED)
10
11 INCLUDE_DIRECTORIES(${CPPTRANSPORT_INCLUDE_DIRS} ${CMAKE_CURRENT_BINARY_DIR})
12
13 ADD_CUSTOM_COMMAND(
14   OUTPUT ${CMAKE_CURRENT_BINARY_DIR}/dquad_core.h ${CMAKE_CURRENT_BINARY_DIR}/dquad_mpi.h
15   COMMAND CppTransport --verbose --fast ${CMAKE_CURRENT_SOURCE_DIR}/dquad.model
16   DEPENDS dquad.model
17 )
18
19 SET(HEADERS ${CMAKE_CURRENT_BINARY_DIR}/dquad_core.h ${CMAKE_CURRENT_BINARY_DIR}/dquad_mpi.h)
20 ADD_CUSTOM_TARGET(Generator DEPENDS ${HEADERS})
21
22 ADD_EXECUTABLE(dquad dquad.cpp)
23 ADD_DEPENDENCIES(dquad Generator)
24 TARGET_LINK_LIBRARIES(dquad ${CPPTRANSPORT_LIBRARIES})
25 TARGET_COMPILE_OPTIONS(dquad PRIVATE -std=c++14 -mavx)
```

The steps involved are:

1. The lines

```
1 CMAKE_MINIMUM_REQUIRED(VERSION 3.0)
2 PROJECT(dquad)
```

are required by CMake. They specify the minimum version of the CMake tool that is required (here version 3.0) and the name of the project being built.

2. The line

```
1 SET(CMAKE_MODULE_PATH ${CMAKE_MODULE_PATH} "~/cppttransport-packages/share/cmake/")
```

should be adjusted to point to the share/cmake directory installed under your installation prefix (see Fig. 2). This will allow CMake to locate the build tools installed by CppTransport.

3. The lines

```
1 SET(CMAKE_CXX_FLAGS_RELEASE "-Ofast -DNDEBUG")
2 SET(CMAKE_C_FLAGS_RELEASE "-Ofast -DNDEBUG")
```

set the compiler flags to be used when building in ‘Release’ mode. Generally it is desirable to optimize CppTransport to *at least* `-O2` or similar, because the templated Boost.odeint steppers require optimization to produce acceptable results. Also, a high optimization setting will encourage the compiler to optimize the automatically-generated C++ produced by the translator. Clang and the Intel compiler produce good results using their `-Ofast` setting, and gcc produces good results using `-O3`. (For the Intel compiler, `-fast` is also a possibility.) The switch `-DNDEBUG` [disables debugging code](#) associated with the `assert()` macro.

4. The next step is to detect the libraries and include files needed by CppTransport. This is managed in a single line:

```
1 FIND_PACKAGE(CppTransport REQUIRED)
```

It was for this command to function correctly that we needed to adjust `CMAKE_MODULE_PATH` above. Specifically, this will detect the SQLite, Boost and MPI libraries required by CppTransport. It will also detect the libraries installed by CppTransport itself.

To make the header files required by these libraries available we use the line

```
1 INCLUDE_DIRECTORIES(${CPPTRANSPORT_INCLUDE_DIRS} ${CMAKE_CURRENT_BINARY_DIR})
```

The variable `CPPTRANSPORT_INCLUDE_DIRS` contains the include paths required by CppTransport and its dependencies. The variable `CMAKE_CURRENT_BINARY_DIR` adds the CMake build directory to the include path, which is done to make the translated core and implementation header files available (see below).

5. Next we must instruct CMake to build the final executable. This is done in two stages: first, we arrange for the model description file `dquad.model` to be translated to the core and implementation headers `dquad_core.h` and `dquad_mpi.h`; and second, we instruct the compiler to process the main file `dquad.cpp` with all the previously-determined include paths and library locations.

- (a) CMake is instructed to invoke the CppTransport translator using an `ADD_CUSTOM_COMMAND()` block,

```
1 ADD_CUSTOM_COMMAND(
2   OUTPUT
3   ${CMAKE_CURRENT_BINARY_DIR}/dquad_core.h ${CMAKE_CURRENT_BINARY_DIR}/dquad_mpi.h
4   COMMAND CppTransport --verbose --fast ${CMAKE_CURRENT_SOURCE_DIR}/dquad.model
5   DEPENDS dquad.model
6 )
```

The `OUTPUT` line advises CMake that this block gives a recipe for constructing the files `dquad_core.h` and `dquad_mpi.h`. The `DEPENDS` line advertises that this recipe depends on the file `dquad.model`, and therefore should be re-run if it is changed. Finally, the `COMMAND` line gives the command to execute; it invokes the CppTransport translator with the options `--verbose` and `--fast`. The CMake variables

`CMAKE_CURRENT_SOURCE_DIR` and `CMAKE_CURRENT_BINARY_DIR` refer to the source and build directories managed by CMake.

- (b) At this stage CMake knows *how* to generate the core and implementation header files, but it does not know that it *should* do so. To instruct it that these files are required, we add a *target* (a deliverable set of objects that CMake can build):

```
1 SET(HEADERS
2   ${CMAKE_CURRENT_BINARY_DIR}/dquad_core.h ${CMAKE_CURRENT_BINARY_DIR}/dquad_mpi.h
3 )
4 ADD_CUSTOM_TARGET(Generator DEPENDS ${HEADERS})
```

This tells CMake that a target called `Generator` depends on the core and implementation header files. If we try to build this target, CMake will invoke the recipe above in order to generate these files.

- (c) Finally, we set up a second target `dquad` that consists of the finished executable and make this depend on the `Generator` target declared above. CMake then knows that the files associated with `Generator` must be built before `dquad`.

```
1 ADD_EXECUTABLE(dquad dquad.cpp)
2 ADD_DEPENDENCIES(dquad Generator)
3 TARGET_LINK_LIBRARIES(dquad ${CPPTRANSPORT_LIBRARIES})
4 TARGET_COMPILE_OPTIONS(dquad PRIVATE -std=c++14 -mavx)
```

The `TARGET_COMPILE_OPTIONS()` command adds extra compiler flags to the `dquad` target. The flag `-std=c++14` is required, because it enables certain C++14 features that are used by the CppTransport platform. Other code generation or optimization options can be specified here; an example is the switch `-mavx` which informs the compiler that it is allowed to generate code using the AVX instruction set extensions available on Intel since Sandy Bridge and on AMD since late 2011/early 2012. Where these instructions are available they can give a useful performance boost.

Depending on your processor, even more recent instruction set extensions may be available such as AVX-2. These extensions have been available on Intel since Haswell, and on AMD they are currently implemented for the Carrizo platform.

If using the Intel compiler to target Intel processors, the switch `-xHost` may be used to indicate that code generation should use all features of the machine being used to build. It is implied by the `-fast` optimization, which is more aggressive than `-Ofast`. Note, however, that `-xHost` should be used with caution if you plan to run executables in a heterogeneous cluster environment because different machines may support different instruction set enhancements. If the executable requires instructions that are not available on the host machine it will terminate with an error message.

The CMake script can be adapted for any CppTransport executable.

Build using CMake.—The build process is the same as for CppTransport itself. First, starting from the directory containing the `CMakeLists.txt` script, create a build directory and move into it:


```
1 mkdir build
2 cd build
```

Next, configure CMake to build using the ‘Release’ configuration.

```
1 cmake .. -DCMAKE_BUILD_TYPE=Release
```

Because it is typically unnecessary to install individual executables the `CMAKE_INSTALL_PREFIX` option can be omitted. However, if you wish to later install your executables to a standard location such as `~/bin` then you can specify a suitable prefix here. Also, if you wish to build with a compiler other than the default then you should specify `CMAKE_C_COMPILER` and `CMAKE_CXX_COMPILER` as in §2.4.

When configuration is complete, the build is initiated by issuing the `make` command. If you then wish to install to a different location, use `make install`. Once the executable has built you may wish to verify that it function correctly by trying the following invocations:

```
1 ./dquad --version
2 ./dquad --models
3 ./dquad --help
```

4.3 Adding an integration task

To make the executable `dquad` useful we must add tasks to generate n -point functions, and also tasks to convert these raw n -point functions into observables. This is done by using the task manager’s `add_generator()` method to inform it that the executable includes specifications for some number of tasks. The `add_generator()` method takes one argument, which should be a callable object accepting a reference to a `transport::repository<>` object as its single argument. `CppTransport` stores all information about initial conditions, parameter choices, tasks, derived products and any generated content in disk-based databases called *repositories*. The `repository<>` class manages these databases and offers related services to other `CppTransport` components.

The first step is always to build some number of integration tasks, because all other tasks depend on the n -point functions that they compute. In this section we illustrate the steps required to build, store and execute a collection of integration tasks.

If you are not familiar with constructing callable objects then a simple option is to use the C++11 *lambda* feature. This is a shorthand way to notate functions. First, declare a function `write_tasks()` that accepts two arguments: a `repository<>` and a model pointer:

```
1 void write_tasks(transport::repository<>& repo, transport::dquad_mpi<>* m);
```

This function should be registered using the `add_generator()` method, by inserting the lines

```
1 // register task writer
2 mgr.add_generator( [=](transport::repository<>& repo) -> void { write_tasks(repo, model.get());
  ↪ });
```

immediately prior to the call to `mgr.process()`.

Advanced usage: Callable objects

The `add_generator()` method accepts any callable, such as a `std::function<>` object. It is not necessary to lambdas if a different solution is preferable. For example, it is also possible supply an instance of any class that provides a call operator `operator()`.

In this implementation, the argument of `add_generator()` is the function

```
[=](transport::repository<>& repo) -> void { write_tasks(repo, model.get()); }
```

This is a lambda expression. It represents an object that behaves as a callable function, taking a single `repository<>` as an argument. The function body is the code enclosed by braces `{ ... }`. It calls the function `write_tasks()`, passing on the `repository<>` object given as its own argument and using the raw model pointer obtained from `model.get()`. For the meaning of the prefix `[=]`, see [here](#).

Building a task.—The final step is to provide a definition for `write_tasks()`. This should construct the integration tasks we want, and store them in the `repository<>` object it is passed.

Integration tasks package together all the information needed to perform a computation of the 2- or 3-point functions. This includes:

- details of the model to be used, identified through the pointer to the model instance passed to `write_tasks()`
- a choice for any parameters used in the Lagrangian, and a value for the Planck mass M_{P}
- a choice for the initial values of the background fields (and optionally their derivatives)
- fixed start and end times for the integration, and a mesh of sample points between these times where samples will be recorded
- a mesh of wavenumber configurations (values of the wavenumber k for the 2-point function, and configurations $\{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3\}$ for the 3-point function) where the 2- and 3-point functions should be sampled

In addition, `CppTransport` provides various options for customizing an integration—for example, by changing the way initial conditions are handled. These options will be described in §5 and are recorded as part of the integration task.

Specifying parameters.—We work with the double-quadratic model as an example. `CppTransport` works in units where $c = \hbar = 1$ but allows us to measure the Planck scale M_{P} using whatever units we find convenient. Typically, however, ‘natural’ units with $M_{\text{P}} = 1$ give good results and in what follows we will make this choice.

The double-quadratic potential (3.1) requires us to specify the mass scales M_{ϕ} and M_{χ} . We will choose $M_{\phi} = 9 \times 10^{-5} M_{\text{P}}$ and $M_{\chi} = 10^{-5} M_{\text{P}}$. A *parameter package* consists of a model, a choice for the Planck mass, and choices for each of the parameters in the Lagrangian. `CppTransport` collects this information using a `transport::parameters<>` object.

Its constructor takes three arguments: the value of the Planck mass; a list of values for the model parameters **in the same order they were declared in the model description file**; and a pointer to the model instance. With our choices we can construct a suitable parameter package using:

```

1 void write_task::operator()(transport::repository<>& repo)
2 {
3     const double Mp = 1.0;
4     const double Mphi = 9E-5 * Mp;
5     const double Mchi = 1E-5 * Mp;
6
7     transport::parameters<> params(Mp, {Mphi, Mchi}, model);
8 }

```

To aid readability it can be helpful to use named temporary variables that give meaning to numbers that are quoted directly. We could have achieved the same effect by writing the single-line construction

```

1 transport::parameters<> params(1.0, {9E-5, 1E-5}, model);

```

but it would then be more difficult to identify the meaning of the numbers.

If it is more convenient, the parameter list can be specified using any suitable iterable container, such as `std::vector<double>` or `std::list<double>` rather than quoting it directly as the initialization list `{Mphi, Mchi}`. If an incorrect number of parameters are passed then `CppTransport` will throw a `std::out_of_range` exception.

Specifying initial conditions.—Next we combine the parameter package with a choice of initial conditions to make an *initial conditions package*. This information is stored in a `transport::initial_conditions<>` object. Its constructor accepts three mandatory arguments: a textual name, which will be used later to refer to this initial conditions package; a parameter package, which specifies the model and parameters to be used; and a list of initial values for the fields. In an N -field model this list can contain either exactly N or exactly $2N$ values:

- if N values are given, `CppTransport` will interpret these as the initial conditions for the background fields **in the order they were declared in the model description**. It will infer initial conditions for the field derivatives using the slow-roll equation $3H\dot{\phi}^\alpha = \partial_\alpha V$, where ∂_α denotes the field derivative $\partial/\partial\phi^\alpha$.
- if $2N$ values are given, these are interpreted as N initial conditions for the background fields ϕ^α (in the same order they were declared) followed by N initial conditions for their derivatives $d\phi^\alpha/dN$ (in the same order as the fields). Here, $dN = H dt$ is a derivative with respect to e-folding number.

As for `parameters`, the value list can be specified using any suitable container or by quoting it directly as an initialization list. If a number of values other than N or $2N$ is given then `CppTransport` will raise a `std::out_of_range` exception.

In addition, the initial conditions package should include information about the time during inflation when these initial field values are intended to apply. This information can be specified in two ways:

- as an initial time N_{init} (specified in e-folds) together with the number of e-folds N_{pre} from N_{init} to the horizon-crossing time of a distinguished scale k_* (at time N_*) that is used as a reference.

- as an initial time N_0 together with the horizon-crossing N_* associated with k_* , and the desired number of e-folds N_{pre} from N_{init} to N_* . This amounts to moving a set of initial conditions specified at N_0 to new initial conditions specified at $N_* - N_{\text{pre}}$.

This version can be used to ‘settle’ a set of field-only initial conditions onto the true dynamical attractor. If the slow-roll approximation holds to reasonable accuracy near the initial time then `CppTransport`’s estimate of the field derivatives will normally be quite accurate. Nevertheless, there will be a period of adjustment while the numerical solution relaxes. This can lead to slight jitter if any n -point functions have initial conditions during this phase.

If adaptive initial conditions are in use (this is normally the recommended configuration; see the discussion on p.68 in §5) then a customized initial condition will be computed for each n -point function. Provided N_{init} is sufficiently early, this customization will automatically allow the initial conditions to relax onto the dynamical attractor. Manual settling is normally required only if N_{init} is very close to the initial time for any n -point function, or if adaptive initial conditions are not being used.

For the purposes of illustration we will set initial conditions for the double quadratic model at $\phi = 10M_{\text{P}}$ and $\chi = 12.9M_{\text{P}}$ and allow `CppTransport` to infer values for the field derivatives. We take the initial time to be $N = 0$ (this is just a convention; any other value of N could be used) and set N_* to occur at $N = 12$. To build an initial conditions package corresponding to these choices we can use:

```

1  const double phi_init = 10.0 * Mp;
2  const double chi_init = 12.9 * Mp;
3
4  const double N_init   = 0.0;
5  const double N_pre   = 12.0;
6
7  transport::initial_conditions<> ics("dquad", params, {phi_init, chi_init}, N_init, N_pre);

```

Remember that when specified in this form, $N_* = N_{\text{init}} + N_{\text{pre}}$. If we had used the second form, perhaps to arrange for some manual settling, the last two parameters `N_init` and `N_pre` would have been replaced by the *three* parameters `N_0`, `N_star` and `N_pre`, corresponding to N_0 , N_* and N_{pre} .

Selecting a mesh of time sample points.—The remaining task is to set up a series of sample points, both for time and wavenumber configuration. To assist in doing so, `CppTransport` provides a mechanism to construct arbitrary meshes that are unions of ranges built using linear or logarithmic spacing. The building blocks of these meshes are objects of type `transport::basic_range<>`. The constructor for this object has the form

```
transport::basic_range<>(lo, hi, N, spacing);
```

It constructs a range of $N + 1$ sample points between `lo` and `hi` (inclusive) that divide the interval $[lo, hi]$ into N parts. The parameter `spacing` should be one of:

- `transport::spacing::linear`: the sample points are spaced linearly
- `transport::spacing::log_bottom`: the sample points are logarithmically spaced from the bottom of the interval

- `transport::spacing::log_top`: the sample points are logarithmically spaced from the top of the interval

If $N = 0$ the range consists of a single value equal to `lo`.

Any number of `basic_range<>` ranges can be composed to produce a composite range. This produces an object of type `aggregate_range<>`. If `A`, `B`, `C` are ranges (which may themselves be composite) then the following are equivalent:

```

1  transport::aggregate_range<> M = A + B + C;
2
3  auto M = A + B + C;
4
5  transport::aggregate_range<> M(A, B);
6  M += C;
7
8  transport::aggregate_range<> M(A);
9  M.add_subrange(B);
10 M.add_subrange(C);

```

It is also possible to construct an empty `aggregate_range<>` by passing no arguments to its constructor. Often it assists readability to use the `auto` type specifier, which informs the compiler that it should deduce an appropriate type for the given assignment.

The ability to construct arbitrary meshes makes it possible to sample certain regions densely and others sparsely. For example, it is possible to sample densely in regions (either of time or wavenumber configuration) that exhibit sharp features while sampling sparsely elsewhere to keep the overall data volume manageable.

For time sampling, a sensible starting point is to sample linearly in N to get a sense of how the correlation functions evolve. Later, the sample mesh can be refined if required. A reasonable starting point might be 300 evenly spaced intervals between the minimum and maximum values of N ,

```

1  const double N_end = 60.0;
2
3  transport::basic_range<> ts(N_init, N_end, 300, transport::spacing::linear);

```

Advanced usage: Arbitrary value types

The `basic_range<>` and `aggregate_range<>` objects are templated and (if needed) can be used to construct a range of values for any numeric type. However, even if you are using a type other than `double` in the integration engine, CppTransport always measures times and wavenumbers using `double`.

Selecting a mesh of wavenumber samples.—Building a mesh of wavenumber samples is similar. For the two-point function, a wavenumber configuration is fixed by the magnitude k . A set of samples can therefore be specified by a range (possibly a composite, as above). The wavenumber $k = 1$ is *defined* to exit the horizon at time $N = N_*$, as determined by the initial conditions package. CppTransport refers to wavenumbers normalized in this way as *conventionally normalized*. When producing derived products it is possible to measure wavenumbers using a number of different normalizations, as will be explained in §4.4.2.

If H is nearly constant then a general wavenumber k will exit the horizon roughly when $N = N_* + \ln k$. This is a good rule-of-thumb when attempting to build a range of k that

covers a given range of e-folds. (When constructing a mesh of ks it is often useful to make use of the logarithmic spacing option in `basic_range<>`.) However, `CppTransport` does *not* assume that H is constant; it calculates the horizon-exit time of each wavenumber exactly.

To begin, we will construct a range of wavenumbers that sample horizon exit times between approximately $N_* + 3.0$ and $N_* + 8.0$:

```
1  const double kt_lo = std::exp(3.0);
2  const double kt_hi = std::exp(8.0);
3
4  transport::basic_range<> ks(kt_lo, kt_hi, 50, transport::spacing::log_bottom);
```

Building 2- and 3-point function integration tasks.—With all of these elements in place, we can proceed to build integration tasks. Currently, `CppTransport` offers two options. While the integration engine can compute the 3-point function for any model, this calculation is expensive. If the 3-point function is not required (perhaps only a power-spectrum analysis is contemplated) then it is much faster to omit it. A task that computes *only* the two-point function is represented by an object of type `transport::twopf_task<>`:

```
1  transport::twopf_task<> tk2("dquad.twopf", ics, ts, ks);
2  tk2.set_adaptive_ics_efolds(5.0);
3  tk2.set_description("Compute time history of the 2-point function from k ~ e^3 to k ~ e^9");
```

Its constructor requires a name, an initial conditions package, a range representing the time sample points, and a range representing the wavenumber samples. Setting a description is optional, but provides a convenient way to document choices including the time- and wavenumber-sampling strategy. The meaning of the `set_adaptive_ics_efolds()` method will be explained in §5.1 below (see p.68).

Alternatively, if we wish to compute the 3-point function, a suitable task can be built using

```
1  transport::threepf_cubic_task<> tk3("dquad.threepf", ics, ts, ks);
2  tk3.set_adaptive_ics_efolds(5.0);
3  tk3.set_description("Compute time history of the 3-point function on a cubic lattice from k ~ e^3 to k ~ e^9");
```

This will sample the three-point function on a cubic lattice (k_1, k_2, k_3) built from the Cartesian product $ks \times ks \times ks$, after filtering out configurations that do not correspond to a physical triangle. Note that this is only one way to construct a 3-point function task. There are other ways to specify the wavenumber configurations to be sampled, including use of Fergusson–Shellard (k_t, α, β) parameters. It is also possible to adjust the default policies that determine which configurations are regarded as physical triangles and whether all configurations produced by the Cartesian product should be retained for integration. These features (and others) are described in §5.3.

To commit these tasks to the repository we use the `commit()` method:

```
1  repo.commit(tk2);
2  repo.commit(tk3);
```

4.4 Running tasks

It is now possible to build the executable, enabling us to experiment with creating repositories and running integration tasks. The source code, as described above, is available from the

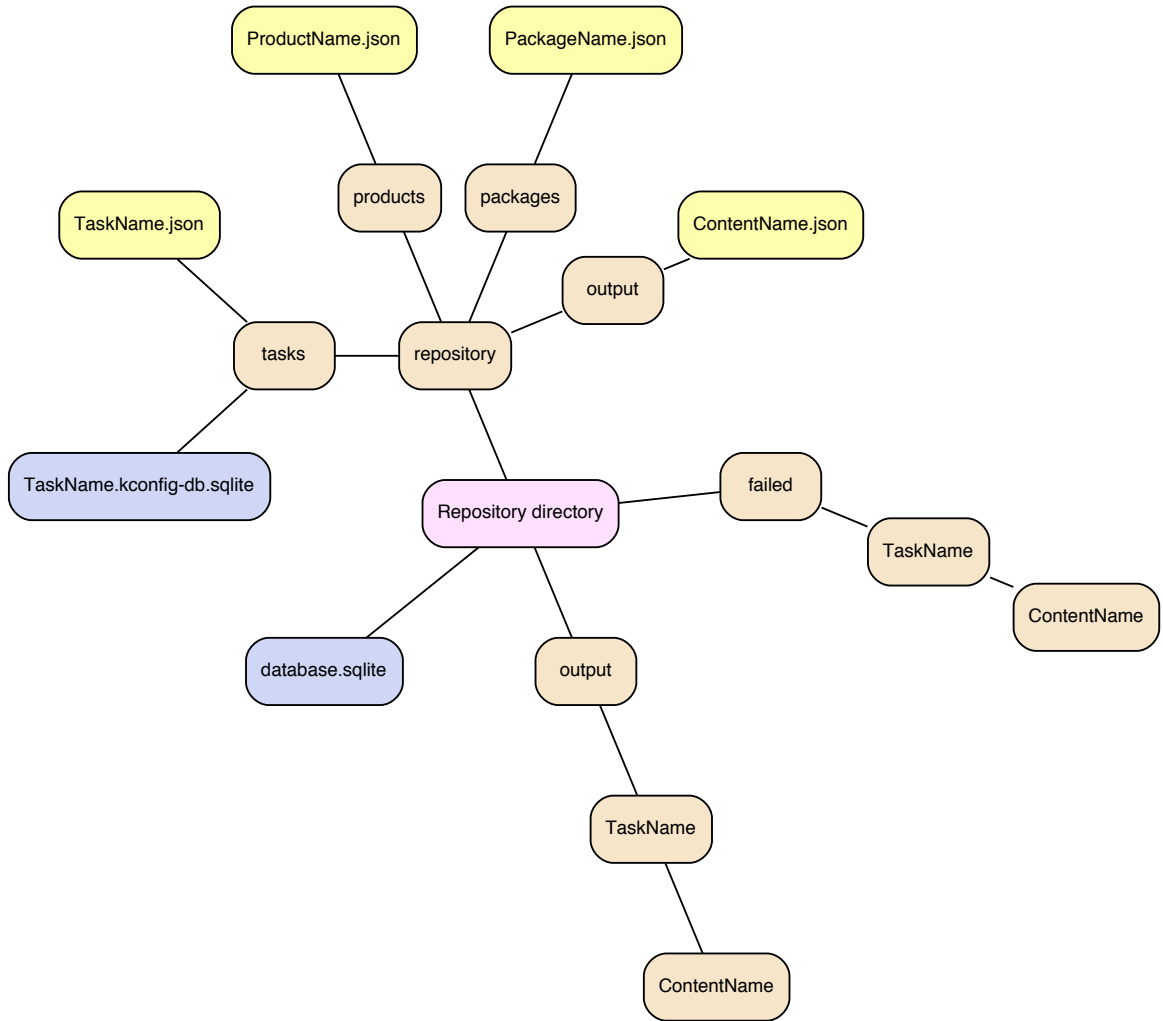


Figure 3. Disk layout of a repository. The node labelled *Repository directory* is the root directory whose name is passed to each `CppTransport` executable.

website <http://transportmethod.com> as `dquad_A.cpp`. If the `CMake` build directory was previously configured correctly then there should be no need to reconfigure. To build, it is sufficient to execute `make`.

4.4.1 Running executables under MPI and creating a repository

The `dquad` executable can be invoked like any compiled object, by passing its name to the shell. Doing so without other arguments will result in `CppTransport` printing the error message ‘Nothing to do: no repository specified’.

Repositories.—In order to carry out practical work it is necessary to specify a repository, using the command line switch `--repo` or its abbreviation `-r`. A repository is a disk-based database managed by `CppTransport`, distributed over a files in a predefined directory structure. The specified repository may already exist, but if not a suitable directory layout will be created; see Fig. 3. Once created, repositories are relocatable and can be moved to different

fling-system locations after creation, or even to a different machine. The *repository directory* is the name passed as the argument of `--repo`. This directory contains up to four items:

- `database.sqlite`. This is a SQLite database that contains summary information describing the relationship between all items in the database—initial conditions packages, tasks, derived products and generated content. The database does not contain full information about these objects; this information is stored as [JSON-format documents](#) elsewhere in the repository, in order that the information they contain is not hidden should it need to be recovered (or processed electronically) without `CppTransport`.

In addition, `database.sqlite` stores information about jobs that are currently running on the repository. This assists in automatically recovering data should there be a crash.

- `repository`. This is a directory containing the JSON documents that describe each repository object in detail.
- `output`. Output generated by tasks is placed in this folder. For a task named *TaskName*, `CppTransport` will generate a subdirectory also called *TaskName*. All content generated by *TaskName* is placed in timestamped folders within this subdirectory.
- `failed`. If an error is encountered while generating output from a task, the log files and other content are placed within this folder for inspection. The organization is the same as for `output`.

The folders `output` and `failed` are created only when needed. A freshly-created repository will contain only `database.sqlite` and `repository`.

The `repository` folder contains further subfolders. As has been explained, these house the JSON documents for each repository record.¹⁰

- `output`. Records describing each group of content generated by a task are stored in this folder in the format `ContentName.json`.
- `packages`. Contains records describing each initial conditions package. A package named *PackageName* is stored as `PackageName.json`.
- `products`. Contains records describing each derived product. A product name *ProductName* is stored as `ProductName.json`.
- `tasks`. Stores records describing each task *TaskName* as `TaskName.json`. For integration tasks, this JSON document is accompanied by a SQLite database with filename `TaskName.kconfig-db.sqlite` storing the list of 2- and 3-point wavenumber configurations to be sampled, together with pre-computed information such as the corresponding time of horizon exit.

Repositories collect groups of related data products, ensuring that their provenance is properly documented and that individual products do not become orphaned. For example, plots

¹⁰If necessary these can be edited by hand, although this practice is not recommended because it loses most of the advantages of a managed repository.

do not become separated from the datasets that were used to produce them, and computations of observables do not become separated from the raw n -point functions and inflationary initial conditions on which they depend.

At the same time, repositories are intended to be a lightweight concept. `CppTransport` allows repositories to be created at will, and does not impose limitations on their use. At one extreme, it would be possible to write all integration tasks, and all generated content, into the same repository. This is probably not a good choice, partly because reporting on the repository (see §4.7.1) will take a long time as the repository becomes large. At the other extreme, every `CppTransport` job could create a new repository. This strategy can work well in practice—especially if used in conjunction with the facility to attach notes to repository records, which can be used to document an evolving series of integrations.

Launching `CppTransport` using MPI.—If using a `CppTransport` executable to create or interrogate a repository, it can be launched as described above in the same way as any other executable. But to execute a task, `CppTransport` expects to be run as a group of related processes communicating within a managed MPI environment. To carry out a task requires at least two processes, but the task manager will make use of as many as are available.

To launch a `CppTransport` executable under MPI, use the following command:

```
1 mpiexec -n 4 dquad --verbose --repo test-repo --create
```

Replace the argument `-n 4` to `mpiexec` by the number of processes you wish to launch; for running tasks it must be ≥ 2 . It is seldom worth launching more processes than there are physical cores to run them on, except for some products that support two threads per core. Intel calls this technology *hyperthreading* and it is available on certain i7 and Xeon processors. Such processors generally identify themselves to the operating system with two times their physical core count. Therefore, normally, it is safe to use whatever number of cores is reported by your machine. In OS X, check Activity Monitor. In Linux the Gnome System Monitor or equivalent performs the same job.

In a cluster environment the argument supplied to `-n` should match the number of cores you request. For example, an Open Grid Scheduler-like job submission script requesting 36 cores managed under OpenMPI might include the lines

```
1 #$ -pe openmpi 36
2 mpiexec -n 36 ...
```

Warning

If you are using `CppTransport` on a network filing system such as NFS or Lustre (which is often the case when running on a cluster), you should add an extra command-line switch `--network-mode` to the `CppTransport` executable.

In order to maximize performance, `CppTransport` enables ‘write-ahead logging’ mode in the underlying SQLite database manager. This gives a significant performance improvement but is not compatible with network filing systems and must be disabled for reliable operation.

4.4.2 Examining the repository wavenumber configuration databases

If the `mpiexec` command given above succeeded, `CppTransport` will have created a repository called `test-repo` in your current working directory. The switch `--create` instructs it to write any available tasks and derived products into the repository by calling each object registered with `add_generator()`. For the example of double-quadratic inflation this is the function `write_tasks()` described in §4.3. The `--create` option should be used only once, the first time that task information needs to be written to the repository. If an attempt is made to commit a second task with the same name as an existing task then `CppTransport` will report an error.

If verbose output is enabled using the switch `--verbose` or `-v` then the constructors of `twopf_task<>` and `threepf_cubic_task<>` will print brief summary information about the tasks that have been constructed. The constructor for `tk2` should print

```

1  dquad.twopf
2  2pf configs: 51           Smallest k: 20.1
3  Largest k: 2.98e+03      Earliest N_exit: N**3.118
4  Latest N_exit: N**8.408  Inflation ends: N=67.78

```

The information given is:

1. the number of 2-point function configurations, here equal to 51 because the `basic_range<>` object `ts` was constructed with $N = 50$ and therefore contains $N + 1 = 51$ points
2. the smallest conventionally-normalized wavenumber sampled by the task, here $k = 20.1 \approx e^3$.
3. the largest conventionally-normalized wavenumber sampled by the task, here $k = 2.9 \times 10^3 \approx e^8$.
4. the earliest horizon exit time, relative to the distinguished time N_* . This will correspond to the smallest wavenumber, which is the largest physical scale. Here, that horizon exit time is ≈ 3.118 e-folds after N_* . This is approximately what we expect from a mode with $k = e^3$, but shows already that the estimate $N_{\text{exit}} \approx N_* + \ln k$ is accurate only to a few percent.
5. the latest horizon exit time, corresponding to the largest wavenumber or smallest physical scale. In this case, the error in the naïve estimate $N_{\text{exit}} \approx N_* + \ln k$ has grown to $\sim 5\%$. Generally these estimates will become worse as the horizon exit time becomes farther from N_* .
6. the time when inflation ends, if `CppTransport` could detect it. By default, `CppTransport` will search for 1000 e-folds from the initial time and attempt to find the point where $\epsilon \equiv -\dot{H}/H^2 = 1$. If it does not find such a point within the 1000 e-fold search window then it will issue a warning, but this does not prevent successful calculation of the n -point functions.

The constructor for `tk3` prints similar information, with the addition of the number of bispectrum configurations that will be sampled:

```

1 dquad.threepf
2 2pf configs: 51          3pf configs: 4017
3 Smallest k: 20.1        Largest k: 2.98e+03
4 Earliest N_exit: N**3.118 Latest N_exit: N**8.408
5 Inflation ends: N=67.78

```

For tasks that sample the 3-point function it is frequently useful to inspect the list of wavenumber configurations that will be computed. There are two ways to do this. The simplest, suitable for tasks that do not sample too many configurations, is to run an HTML report on the repository. This writes details of the tasks into an easily-browsable HTML document. The second option is slightly less simple but better suited to tasks that sample a large number of configurations. The list of sample points is written into SQLite databases held in the repository/tasks directory, and these can be inspected directly using a suitable tool.

Option 1: examine configurations using an HTML report.—This option is generally preferred if the task samples fewer than 5000 configurations. The HTML report generator does not include a wavenumber listing for tasks with more than 5000 wavenumber configurations because it makes the report too large: HTML documents are not the best way to examine such a large database.

To produce a report for the repo-test repository that has just been created, execute

```

1 ./dquad --repo test-repo --html test-report

```

This will create a report in the directory test-report. In a desktop environment the report can usually be viewed by opening the file test-report/index.html, for example by a double-click. The report is divided into a number of tabs, most of which will be disabled at this stage because the repository contains only integration tasks—there are no tasks of other types, or any generated content. However, it should be possible to see details of the **dquad** initial conditions package under the ‘Packages’ tab, and the **dquad.twopf** and **dquad.threepf** tasks under the ‘Integration tasks’ tab. The report for each task will include the number of 2- and 3-point wavenumber configurations that are to be sampled. Next to this number is a link labelled ‘show’. Clicking this link will display an overlay listing the wavenumber configurations as a table; see Fig. 4.

The drop-down menu in the top left can be used to adjust the number of configurations displayed per page, and the position indicator in the bottom right can be used to move through the available pages. Clicking the arrows in the table header will sort the table in ascending or descending order on the corresponding column. The information displayed for both configurations of the 2- and 3-point functions (‘2pf configurations’ and ‘3pf configurations’) is:

- **Serial.** This is a unique serial number identifying the configuration.
- **Wavenumber k .** For configurations of the 2-point function this is the conventionally-normalized magnitude k . For configurations of the 3-point function it is the conventionally-normalized value of $k_t = k_1 + k_2 + k_3$, which is the perimeter of the triangle formed by the momenta \mathbf{k}_1 , \mathbf{k}_2 , \mathbf{k}_3 .
- **Horizon-exit time t_{exit} .** For 2pf configurations this is the time (measured in e-folds) when $k_{\text{com}} = aH$. Here, k_{com} is a *comoving* wavenumber. Comoving wavenumbers are

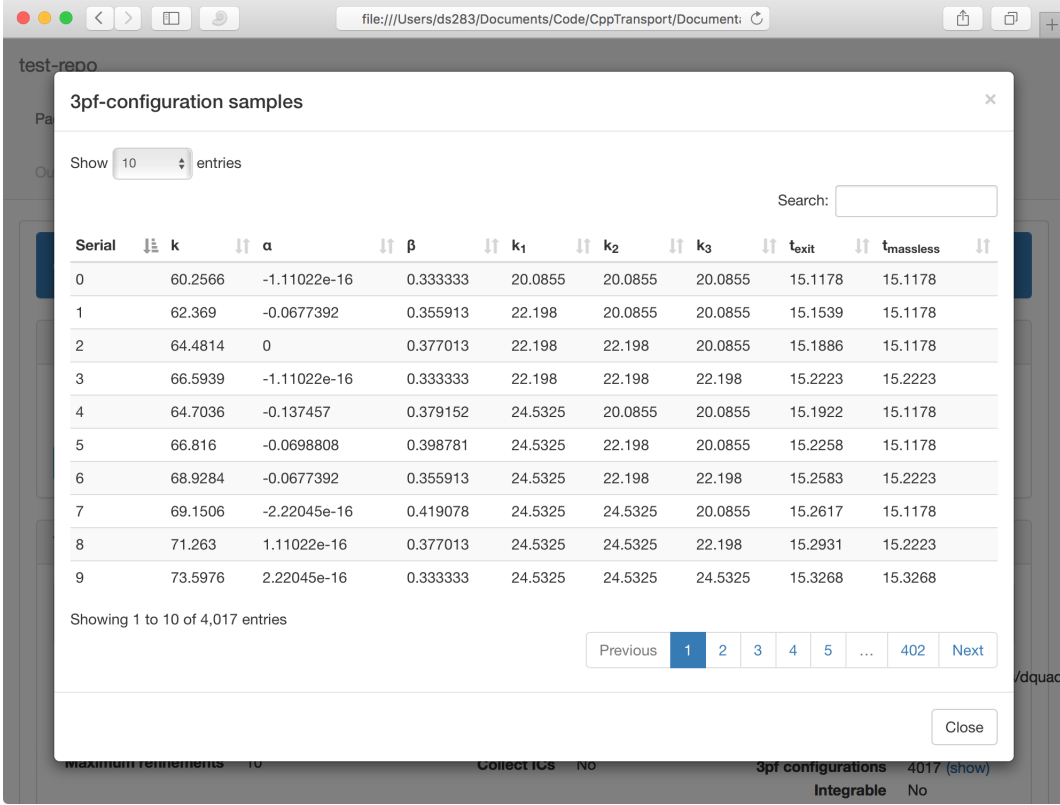


Figure 4. Viewing the sampled 3-point function wavenumber configurations in an HTML report.

computed from conventionally-normalized wavenumbers by adjusting their normalization so that the conventional wavenumber $k = 1$ satisfies $k_{\text{com}} = a_* H_*$ at time N_* . For 3pf configurations there is no unique concept of horizon exit time because the wavenumber associated with each side of the momentum triangle can exit at different times. The time reported as t_{exit} is the average time in the sense $k_t = aH$, where here k_t is comoving-normalized.

If CppTransport is unable to compute the horizon exit time for all configurations (presumably because for at least one configuration it occurs *before* the initial time) it will issue an error:

```
dquad.twopf: extreme values of N did not bracket time of horizon exit; check whether range of N
↔ contains horizon exit times for all configurations
```

To fix this it is usually necessary to move the initial time earlier while keeping the horizon exit time of the longest mode constant, or vice versa.

- **Massless time t_{massless} .** In order to apply suitable initial conditions, CppTransport computes a *massless time* t_{massless} for each 2pf configuration. This is defined to be the time when $(k/a)^2 = M^2$ where M^2 is the largest eigenvalue of the mass matrix $M_{\alpha\beta}$, or the time of horizon exit if it is earlier.

For 2pf configurations the quoted time is the massless time computed according to this prescription. For 3pf configurations it is the earliest massless time associated with the individual wavenumbers \mathbf{k}_1 , \mathbf{k}_2 , \mathbf{k}_3 . This is used when determining where to set initial conditions for a 3pf configuration.

If CppTransport is unable to compute the massless time for all configuration it will issue an error similar to that for the horizon-exit time:

```
dquad.twopf: extreme values of N did not bracket massless point; check whether range of N
↪ contains massless time for all configurations
```

In addition, the table of 3pf configurations includes some extra columns:

- **Shape parameters** α , β . Sometimes it is useful to measure the shape of the momentum triangle using the parameters α , β introduced by Fergusson & Shellard [53]. They are defined by

$$\alpha = \frac{2(k_1 - k_2)}{k_t} \tag{4.1}$$

$$\beta = 1 - \frac{2k_3}{k_t}.$$

These values are reported for each configuration.

- **Side lengths** k_1 , k_2 , k_3 . The comoving side lengths are also reported.

Option 2: inspect the SQLite databases directly.—If the table of sample configurations is large, or if there is a requirement to inspect subsets of the list, it is better to view the table in a dedicated SQL database management tool. Many such tools exist. The simpler tools are intended to manage only SQLite databases. [Sqliteman](#) is an example of this type. It is packaged with Ubuntu, and can be installed on OS X using [MacPorts](#) or [Homebrew](#). More complex tools are capable of managing many different types of database, and these are often more powerful at the expense of a more complex user interface. The free tool [DBeaver](#) is an example in this category. Another is [DataGrip](#); this is a commercial product, but free licenses are available to academic users.

The wavenumber configuration databases can be found in the directory repository/tasks within the repository. The database for a task named *TaskName* is *TaskName.kconfig-db.sqlite*. Opening this file in a database manager will reveal a table named `twopf_kconfig` for a task sampling only the 2-point function, and two tables named `twopf_kconfig` and `threepf_kconfig` for a task that also samples the 3-point function. These tables list the data described above, in addition to some columns that are not displayed in the HTML table. First, each wavenumber k or k_t is listed twice with conventional and comoving normalizations. Second, there are extra columns with names beginning `store_`. These are used internally by CppTransport and can be ignored.

For 3pf configurations, the table is normalized in the sense that the k_1 , k_2 , k_3 side lengths are not included directly but refer to the serial number of the corresponding entry in the 2pf configuration table. This helps to ensure that the database remains internally self-consistent. To display a table that lists the side lengths explicitly requires an SQL query:

```

1 SELECT
2   threepf_kconfig.serial      AS serial,
3   threepf_kconfig.kt_conventional AS kt_conventional,
4   threepf_kconfig.alpha      AS alpha,
5   threepf_kconfig.beta       AS beta,
6   threepf_kconfig.t_exit_kt   AS t_exit_kt,
7   w1.conventional            AS k1_conventional,
8   w2.conventional            AS k2_conventional,
9   w3.conventional            AS k3_conventional,
10  threepf_kconfig.t_exit_kt   AS kt_exit_kt,
11  threepf_kconfig.t_massless  AS t_massless
12 FROM threepf_kconfig
13 INNER JOIN twopf_kconfig AS w1 ON w1.serial = threepf_kconfig.wavenumber1
14 INNER JOIN twopf_kconfig AS w2 ON w2.serial = threepf_kconfig.wavenumber2
15 INNER JOIN twopf_kconfig AS w3 ON w3.serial = threepf_kconfig.wavenumber3
16 ORDER BY serial;

```

4.4.3 Launch and track tasks from the command line

If the set of 3pf sample configurations has been constructed correctly the next step is to ask CppTransport to carry out the tasks. A CppTransport executable can be instructed to perform as many tasks as are desired, in which case it will perform them sequentially. To launch it with 4 processes, carrying out both the `dquad.twopf` and `dquad.threepf` tasks, we would use

```
1 mpiexec -n 4 dquad -r test-repo --task dquad.twopf --task dquad.threepf
```

While the job is in progress, executing the command

```
1 ./dquad -r test-repo --inflight
```

will show details of the tasks being processed:

In-flight content:							
Name	Task	Type	Initiated	Duration	Cores	Completion	
20160516T123513-1	dquad.threepf	integration	2016-May-16 12:35:13	33s	4	--	

For each ‘in flight’ task,¹¹ the information shown comprises:

- The **group name**. CppTransport refers to the output produced by each execution of a task as a *content group*. For an integration task the content group will consist of a database containing various tables for the n -point functions and associated data products. For the post-processing tasks currently available—to compute n -point functions of ζ , and to take inner products with the bispectrum—the content group will consist of further databases containing these quantities. For output tasks the content group will contain plots, tables or Python scripts.

Each content group is given a unique name derived from its timestamp. The format is `yyyymmddThhmmss` where `yyyy` is replaced by the year, `mm` by the month, and so on. The capital `T` separates the date from the current time.

If two tasks happen to be initiated close together, their time stamps may clash. In this case CppTransport will append `-N` to the group name, where N is a unique number. The repository database is designed to be safe when used by multiple processes, so name

¹¹Only those tasks that are currently active are shown in this list. Although we specified two tasks on the command line, CppTransport processes them sequentially and therefore only one at once will appear in the list.

collisions will not occur even if different `CppTransport` jobs attempt simultaneously to generate a content group in the same repository.

- The **task name** and **task type**. This identifies the task to which the content group belongs.
- The **job start time** and **duration**. For long-running jobs, this enables you to keep track of the total elapsed time.
- The **number of cores** used by the job.
- An **estimated time of completion**. For long-running jobs, `CppTransport` will attempt to estimate when the job will complete on the assumption that the items it has processed so far are typical. `CppTransport` keeps track of the time required to process each item of work—for example, to integrate a single configuration of the 2- or 3-point function, or to generate a plot. The completion time is estimated assuming the time taken to process each remaining work item will be the current average time-per-item. This estimate is often accurate but can be misleading if the remaining work items are atypically expensive to compute.

The time-to-completion estimate is first generated after 5 minutes. After this, it is updated at intervals of 10% of the total number of work items. If verbose mode is enabled then `CppTransport` will simultaneously print a brief advisory message summarizing progress so far. For the double quadratic example, on most modern hardware, both 2- and 3-pf integrations will complete before `CppTransport` generates any progress update.

If verbose mode is enabled, `CppTransport` will emit brief updates as it works through the list of tasks. For the `dquad.twopf` and `dquad.threepf` tasks of double quadratic example its output will be similar to:

```
Task manager: processing task 'dquad.twopf' (1 of 2)
Committed content group '20160516T123513' for task 'dquad.twopf' at 2016-May-16 13:35:13
Task manager: processing task 'dquad.threepf' (2 of 2)
Task manager: 2016-May-16 13:40:29
Items processed: 3229 In flight: 496 Remaining: 292
Complete: 80.4% Mean CPU/item: 0.249s Assignment: 60s
Estimated completion: 2016-May-16 13:41:46 (1m 17.2s from now)
Task manager: 2016-May-16 13:41:26
Items processed: 3826 In flight: 181 Remaining: 10
Complete: 95.2% Mean CPU/item: 0.277s Assignment: 60s
Estimated completion: 2016-May-16 13:41:44 (18.6s from now)
Task manager: 2016-May-16 13:41:36
All work items processed: 2016-May-16 13:41:36
Committed content group '20160516T123513-1' for task 'dquad.threepf' at 2016-May-16 13:42:06
Task manager: processed 2 database tasks in wallclock time 6m 53s | time now 2016-May-16 13:42:06
```

Notice that—in this case—the 2pf task `dquad.twopf` completed so quickly that the content group from the second task `dquad.threepf` has the same timestamp; the timestamp itself is measured using [UTC](#). As explained above, to keep the names unique `CppTransport` has renamed the second group `20160504T202210-1`.

To confirm that output from these groups has been safely written to the repository, use the `--status` switch:

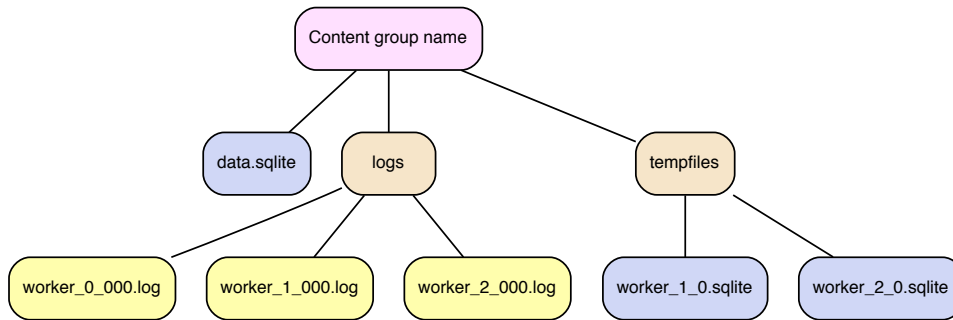


Figure 5. Directory structure for an integration content group. The `tempfiles` directory is present only while this content group is in flight; it is removed when the content group is committed to the repository.

```
1 ./dquad -r test-repo --status
```

This causes `CppTransport` to display a short summary of the tasks available in the repository, and the number of content groups associated with each task. In this case the output should be:

```
Available tasks:
Task          Type          Last activity  Outputs
dquad.threepf integration  2016-May-16 12:42:06    1
dquad.twopf   integration  2016-May-16 12:35:13    1
```

If any tasks are still in flight then `--status` will additionally display the same information shown by `--inflight`.

4.5 What happens while an integration task is in progress

Now let us consider what happened while each integration task was in progress. At the outset, when `CppTransport` comes to process each new task, it acquires a unique content group name derived from the current time. A folder with this name is created in the output directory of the repository, under a subdirectory corresponding to the name of the owning task.

Each content group directory has the structure shown in Fig. 5. There are three items at the top level:

- A SQLite database named `data.sqlite`. This is the main data container that stores the output produced by the job. It is just a normal SQLite database, so it can be inspected using the database management tools described in §4.4.2.
- A directory named `logs`. This contains fairly verbose logs describing the activity of each process while the job was active. Each process generates a logfile named `worker_N_yyy.log` where N is a number identifying the process—the master has $N = 0$ and the workers have $N > 0$ —and yyy is a unique suffix that is usually `000`.

Often it is unnecessary to inspect the logs, but they provide useful information if an integration task is not behaving as expected.

- A directory named `tempfiles`. This is used only while the task is in flight, and contains temporary SQLite databases into which each worker writes its results. The master

process aggregates data from these databases into the main container `data.sqlite`. This has the effect that *only the master process* writes to the main container.

The temporary databases are removed when their contents are merged with the main database. Once the task is complete and the content group has been committed to the repository, the `tempfiles` directory is removed.

A typical integration will involve the following sequence of steps.

1. The task manager running on the master process begins work on a new integration task. It sends messages to the worker processes, instructing them to prepare for integration activity associated with this task.
2. Once all workers have signalled that they are ready, the task manager issues a small number of work items to each worker. For integration tasks these work items are individual wavenumber configurations. The workers process these configurations and report the time taken. The results of each integration are held in memory on each worker.
3. The task manager on the master process attempts to balance the workload of each worker by using the reported times to estimate capacity. It estimates the number of configurations each worker can process in 60 seconds and then issues a corresponding number of work items, modified if necessary to prevent any one worker consuming an unbalanced fraction of the queue. The effect is that slower cores will be issued with fewer work items, and faster cores will be issued with more.

As the workers process each group of work items, they report the time taken back to the master. This information is used to update the estimate of each worker's capacity and to adjust future work allocations.

4. The workers process integrations as they arrive, retaining the results in memory. To prevent memory requirements rising unboundedly, each worker is given a fixed capacity. When the accumulated integration produces outgrow this capacity they are flushed to a temporary database in the `tempfiles` directory. (This strategy is adopted for performance reasons. It is faster to write the database to disk in one go, rather than writing the data piecemeal at the end of each integration.)

The worker process then sends a message to the master, asking for this temporary database to be aggregated into the main container.

5. The master process continues to issue new work and aggregate temporary databases. For large databases and some choices of filing system (especially slow network storage) the aggregation time may become lengthy, in which case the task manager will adjust the number of work items it allocates to each worker in an attempt to prevent workers waiting for new work allocations while an aggregation is in progress.
6. Eventually all work items have been processed and their results aggregated into the main container. At this point the task manager performs an integrity check that attempts to detect any missing items. It then generates a repository record for the content group. If the integrity check was successful the group is marked as complete.

Only complete groups can be used to generate subsequent derived products. However, incomplete groups are retained in the repository because their data can be re-used. Finally, the `tempfiles` folder is removed.

4.6 Using checkpoints and recovery to minimize data loss

The amount of memory available to each worker can be adjusted using the command-line option `--caches`. It should be followed by an argument representing the cache size as an integer number of megabytes. The default cache size is 500 Mb.

Generally, it is advantageous to keep the cache size fairly large. A small cache size will encourage the workers to flush their temporary databases frequently, which can generate a large amount of disk activity. If the master process is busy with aggregations then some workers may stall while they wait for new work items to arrive. A large cache mitigates this, at least if the main container does not become too large, because a small number of large aggregations tends to be faster than a large number of small aggregations.

On the other hand, the total cache memory allocated to cache should not become larger than the physical memory available on a machine. This will usually cause some physical memory to be swapped out to disk, potentially slowing down the progress of the job.

Advanced usage: Estimating cache requirements with paired tasks

For paired post-integration tasks it should be remembered that each task uses an independent cache. While the data generated by post-integration tasks is usually smaller than an integration task, the cache size should be chosen to prevent out-of-memory problems.

With the default cache size of 500 Mb, a 4-process job could consume up to 1.5 Gb for integration-only tasks or 3 Gb for a paired set. An 8-process job would consume up to 3.5 Gb for integration-only or 7 Gb when paired. If running on laptop- or desktop-class hardware these numbers should be adjusted to ensure that memory requirements stay within bounds. Similar calculations apply if running in a cluster environment.

If the cache is large then a significant amount of data can accumulate in memory before being written to disk. In ordinary execution this does not an issue. However, if problems occur then this situation is undesirable: in the event of a crash, all data will be lost and would need to be expensively regenerated. The same applies to long-running tasks on a cluster, where jobs may be terminated by the scheduler, or the machine restarted, in a way that is beyond the control of individual users.

To mitigate these risks `CppTransport` offers the option to set checkpoints for each task at fixed time intervals. At the first opportunity after a checkpoint, a worker will flush its cache to a temporary database and ask the master process to aggregate it. If the job is subsequently terminated—by a crash, machine restart, or other cause—then any information stored in the main container can be recovered and used to *seed* another task. In this way the CPU effort spent performing successful integrations is not wasted.

To set checkpoints, the command-line option `--checkpoint` is used. It should be followed by a time interval measured as an integer number of minutes. Exactly what interval is appropriate will depend on the typical time taken to integrate a configuration, but could perhaps be 30 to 60 minutes. Unless each integration takes substantially longer than this,

the result is that no more than ~ 1 hour of work would need to be regenerated following a crash.

Advanced usage: Setting default checkpoints for a task

In addition to the global checkpointing interval set by `--checkpoint`, it is possible to set default checkpoint intervals for each task using the `set_default_checkpoint()` method of an integration task; see §5.1. Each task may set a different default checkpoint interval.

If an explicit checkpoint interval is given on the command line, it overrides any task-specific defaults.

Example.—We can simulate a crash by manually terminating the `dquad` executable. Start a new instance of the `dquad.threepf` task by typing

```
1 mpiexec -n 2 dquad -v -r test-crash --create --checkpoint 1 --task dquad.threepf
```

This starts a `CppTransport` job using only two processes—a master and a single worker. It will therefore proceed more slowly, giving time to interrupt it. The checkpoint interval has been set to 1 minute, and the job output will be written into a new repository called `test-crash`. Monitor progress using a separate terminal and the `--inflight` option. After the job has been in progress for a few minutes use `Ctrl-C` to terminate it.

Even after termination, using `--inflight` will appear to show that the task is still underway; by itself the repository database has no way to know that a crash has occurred:

```
1 $ ./dquad -r test-crash --inflight
2 In-flight content:
3 Name          Task          Type          Initiated    Duration    Cores    Completion
4 20160505T112925 dquad.threepf integration 2016-May-05 11:29:25 3m 41s    2        --
```

To deal with this situation we should use the command-line switch `--recover` to inform the repository that the integration is no longer live, and recovery should be attempted. `CppTransport` informs us about each content group it is able to recover:

```
1 $ ./dquad -v -r test-crash --recover
2 Committed content group '20160506T093816' for task 'dquad.threepf' at 2016-May-06 10:40:44
3 Warning: Content group '20160506T093816' has missing content
```

The recovery process may take some time. `CppTransport` must ensure that the database is left in a consistent state and this can entail relatively costly comparison between the various tables held in the database container.

Currently, recovery is a global repository operation. When `--recover` is specified, `CppTransport` will perform recovery for all tasks that are currently registered as in-flight. If you have multiple tasks running against the same repository and need to perform recovery, you may wish to wait until no more active tasks remain or manually terminate the remaining active processes.

Seeding an integration from a recovered content group.—Normally, after successful recovery, the next step would be to restart the task, recycling any successful results from the recovered content group. To do this we instruct `CppTransport` to use the recovered group as a *seed*, using the `--seed` switch followed by the name of the content group to use:

```

1 $ mpiexec -n 4 dquad -v -r test-crash --seed 20160506T093816 --task dquad.threepf
2 Committed content group '20160506T094106' for task 'dquad.threepf' at 2016-May-06 10:42:38
3 Task manager: processed 1 database task in wallclock time 1m 31.9s | time now 2016-May-06
  ↪ 10:42:38

```

CppTransport will copy any successful work items from the seed content group, and then organize the worker processes to compute whatever items remain outstanding. There is no limit to how many content groups can be chained together by this process of recovery followed by seeding.

Once the seeded integration completes, CppTransport's `--status` report shows (as expected) that two content groups are now attached to the `dquad.threepf` task:

```

1 $ ./dquad -r test-crash --status
2 Available tasks:
3 Task          Type          Last activity  Outputs
4 dquad.threepf integration  2016-May-06 09:42:38    2
5 dquad.twopf   integration  2016-May-06 09:38:16    0

```

To obtain more information on these groups, use the `--info` switch followed by the task name:

```

1 $ ./dquad -r test-crash --info dquad.threepf
2 dquad.threepf -- integration task
3 Created: 2016-May-06 09:38:16      Last update: 2016-May-06 09:42:38
4 Runtime version: 2016.1
5 Task type: threepf
6 Initial conditions package: dquad
7 k-config database: repository/tasks/dquad.threepf.kconfig-db.sqlite
8
9 Task description
10 Compute time history of the 3-point function on a cubic lattice from  $k \sim e^3$  to  $k \sim e^9$ 
11
12 Content group          Created          Last update  Complete  Size
13 20160506T093816      2016-May-06 09:40:42  2016-May-06 09:40:44    No    4e+02 Mb
14 20160506T094106      2016-May-06 09:41:06  2016-May-06 09:42:38    Yes   9.1e+02 Mb

```

The `--info` switch can be used with the name of any repository object. It prints similar information to that shown by an HTML report, but can be more convenient for quick inspection of individual records.

Here, the table at the bottom gives a short summary of the two content groups. Notice that the interrupted group is marked as incomplete. The reported size corresponds to the disk space occupied by the data container `data.sqlite`. For the final group (here `20160506T094106`) this is just under 1 Gb, showing that the generated datasets can become large even with a modest number of bispectrum configurations and a few hundred time sample points.

CppTransport tracks the relationship between different content groups. Inspecting the repository record for `20160506T094106` shows that `20160506T093816` was used as a seed:

```

1 $ ./dquad -r test-crash --info 20160506T094106
2 20160506T094106 -- integration content
3 Created: 2016-May-06 09:41:06      Last update: 2016-May-06 09:42:38
4 Runtime version: 2016.1          Task: dquad.threepf
5 Type: threepf                    Locked: No
6 Tags: --
7
8 Complete: Yes
9 Workgroup: 1
10 Seeded: Yes
11 Data type: double
12 Seed group: 20160506T093816
13 Has statistics: Yes
14 Initial conditions: No
15 Size: 9.1e+02 Mb
16 Container: output/dquad.threepf/20160506T094106/data.sqlite
17
18 Metadata
19 Wallclock time: 1m 20s
20 Total time: 6m 22.3s
21 Min integration: 0.0329s
22 Max integration: 4.55s
23 Configurations: 3188
24 Failures: 0

```

When complex relationships exist between different content groups, it becomes difficult to navigate the repository using `--info` from the command line. In such cases it is often more convenient to generate an HTML report that summarizes the repository contents. We used these reports in §4.4.2 to examine the wavenumber configurations sampled as part of each integration task, but they have many other uses.

Generating a report is done as in §4.4.2,

```

1 ./dquad --repo test-repo --html test-report

```

Now open `test-report/index.html` in a web browser and use the ‘Integration content’ tab to view records for each content group. For the seeded group, the record includes the name of seed but this is also hyperlinked—clicking on its name will take you directly to its record. Likewise, it is possible to click the task name to view its details. See Fig. 6.

4.7 How is the integration time spent?

4.7.1 Using HTML reports to analyse integration performance

It is often useful to understand what determines the total execution time for an integration task, especially if performance is different from what would be expected. This can happen in two ways. First, the combination of batch size, aggregation frequency and number of processes can accidentally trigger an excessive number of stalls, where the workers spend a long time idle because the master is too busy to issue them with work. To detect this kind of scenario the most helpful tool is the process Gantt chart described in §4.7.2 below.

Second, the integration time per configuration can vary significantly. The total execution time therefore depends strongly on the range of configurations included in each task. A typical use of `CppTransport` would be to sparsely sample a range of configurations (k_1, k_2, k_3) in an exploratory step, before increasing the number of sample points to perform some specific science analysis—for example, to predict the CMB temperature bispectrum from a specific inflationary model. Before stepping up to a more dense set of sample configurations it is

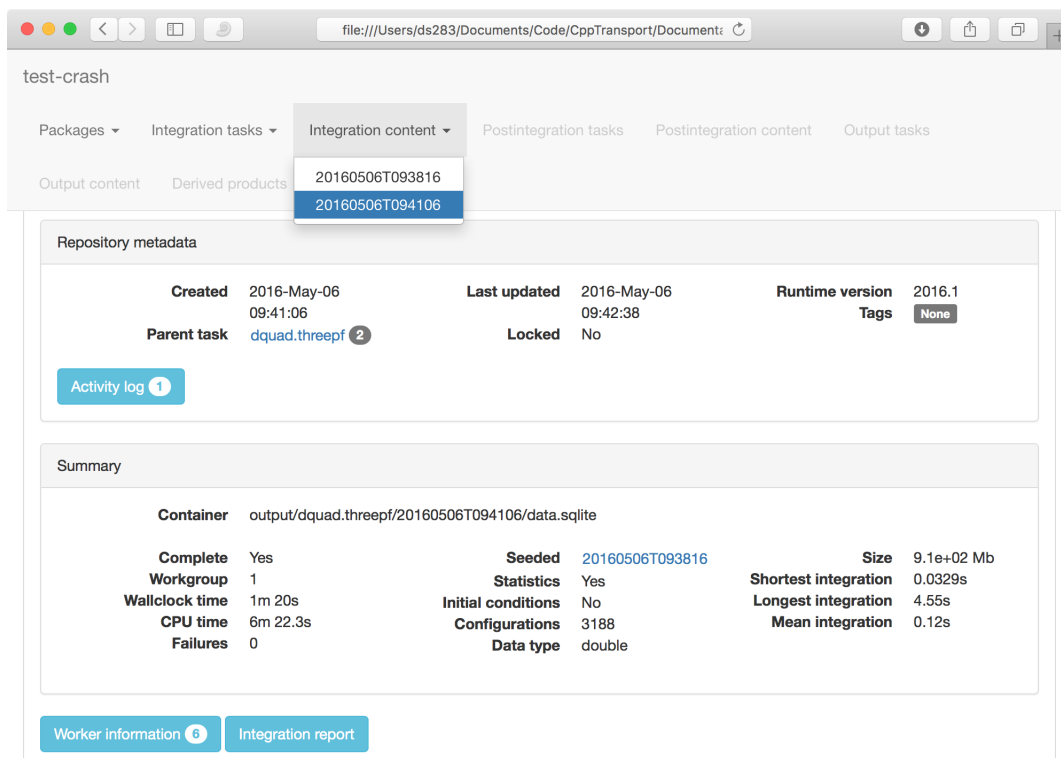


Figure 6. HTML report for seeded content group. Notice that group relationships are hyperlinked, so it is possible to click on the name of the attached seed group to view its record. The same is true for the task names and any other repository objects.

very helpful to be aware of the way in which integration time depends on configuration. The information needed to understand this scaling is included in an HTML report.

Worker information table.—Under the ‘Integration content’ tab, the report for each content group includes two blue buttons near the bottom. One is labelled ‘Worker information’, and clicking it will toggle a table listing each worker process that has contributed to the content group; see Fig. 7. The table identifies each worker by a pair of coordinates (w, n) , where w is the *workgroup number* and n is the *worker number*. When a new content group is created its workers are assigned workgroup number 0. If this group is subsequently used to seed another group then the workers in the second group are assigned workgroup number 1, and so on. The worker number identifies a unique worker within the workgroup.

For each worker, the table lists:

- the hostname of the machine on which this worker was running. This can help identify problematic machines, especially in a cluster environment.
- the type of backend in use. In current versions of CppTransport, as explained in §3.2, this will be the MPI implementation.
- the steppers used for integration of the background and perturbations, and the tolerances applied in each case. The tolerances are given in the format (abserr, relerr).

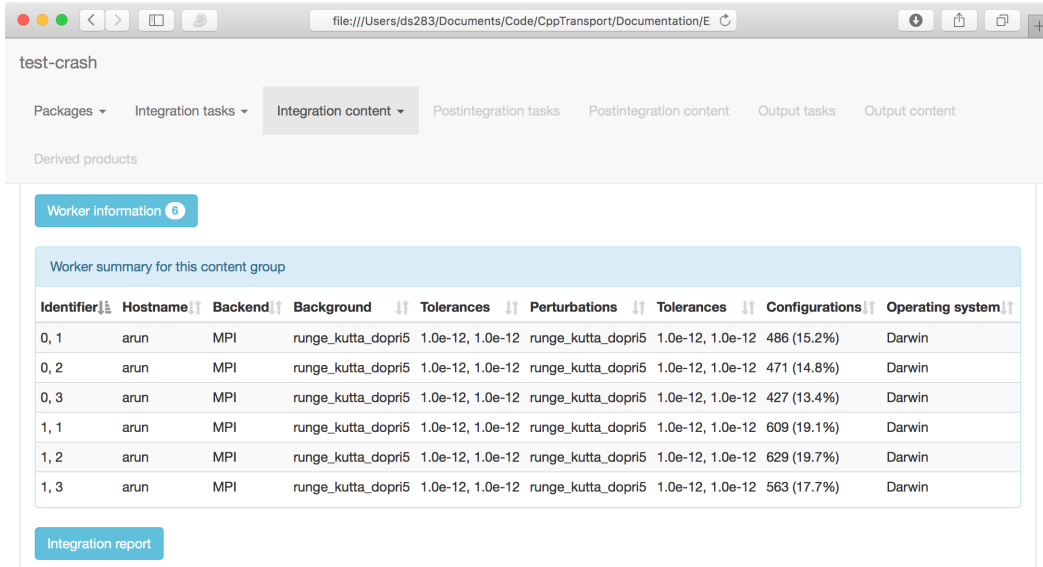


Figure 7. Worker information table displayed as part of a content group record.

- the number of configurations processed by the worker, both in total and as a percentage of the task.
- the operating system on which CppTransport was running.

Integration report.—The second blue button is labelled ‘Integration report’. Clicking it toggles a set of summary plots.

- For any kind of integration task the report includes a bar chart showing the number of configurations processed by each worker, and a histogram showing the distribution of integration times within the task. For the 3-point function of the double quadratic model this distribution is shown in Fig. 8; it is roughly a power law. This is fairly typical for CppTransport tasks that sample a range of different configurations: most configurations integrate relatively quickly (here $\lesssim 0.1$ s), but there is a heavy tail of rare configurations that take much longer (here, a few $\times 10^0$ s). These expensive configurations are usually those that probe the squeezed limit of the 3-point function.
- For tasks that sample the 3-point function, CppTransport includes extra plots showing configuration dependence of the integration time (Fig. 9). In smooth models where the bispectrum does not exhibit features, and assuming use of adaptive initial conditions (§5.1), the strongest dependence is usually on the squeezing parameter k_3/k_t , where k_3 is taken to be the shortest side of the momentum triangle. This is clearly visible in the top two plots of Fig. 8. In the k_t plot (top-left panel) there are a range of integration times for each k_t , with the range widening as k_t increases. However, the colour-bar shows that configurations generating the longest integration times have small k_3/k_t . The k_3/k_t plot (top-right panel) gives the same conclusion in a different form. The dependence on k_3/k_t is an approximate power law where the squeezing is significant.

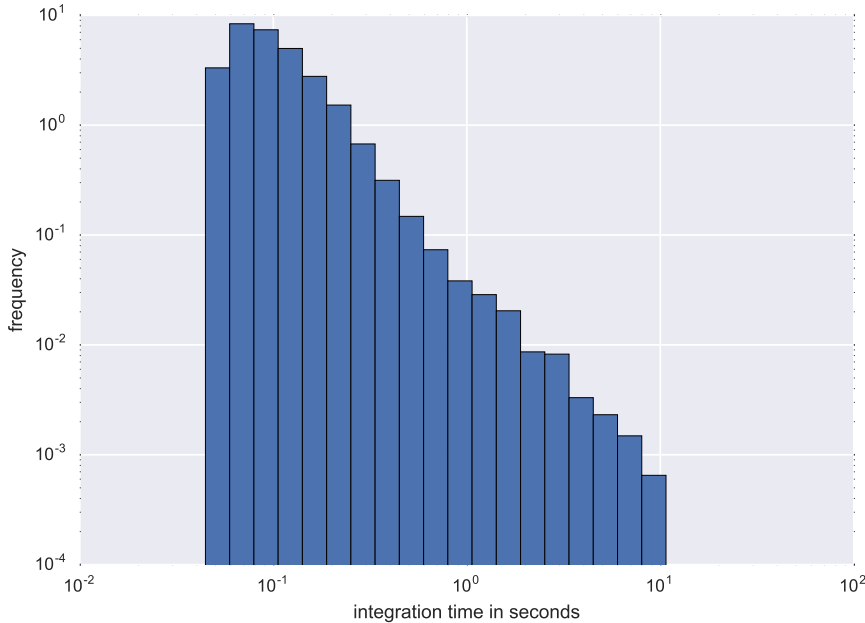


Figure 8. Distribution of integration times for the three-point function in the double quadratic model constructed in §4.3.

4.7.2 Generating a Gantt chart of worker activity

The integration report shows how the intrinsic computation cost scales with configuration, and helps identify regions where it is cheap or expensive to add configurations. These scalings are set partly by the nature of the problem, partly by detailed microphysical interactions determined by each specific model, and partly by the integration scheme employed by `CppTransport` and its use of ‘transport’ or evolution equations.

These intrinsic scalings are one factor contributing to the overall numerical efficiency achieved by `CppTransport`. The remainder is determined by how effectively the master process is able to feed tasks to its workers. `CppTransport` tries to adjust its scheduling strategy to respond to environmental pressures. It is frequently successful but under some circumstances the master process may become overwhelmed, meaning that new batches of work are not allocated to workers in a timely fashion. This leads to workers idling while they wait for new work, described as a ‘stall’. For this reason it can be useful to check what the workers are doing, and in particular whether progress is being inhibited by stalls.

To detect stalls, the most useful tool is the process Gantt chart. Specifying the option `--gantt` on the command line will cause `CppTransport` to produce a Gantt-like timeline showing the activity of each worker. Bars are colour-coded according to the type of activity, and a legend is included identifying each colour. The `--gantt` option should be followed by a filename, and the output format will be determined by its extension. Any format supported by the `Matplotlib` backend can be used, of which the most useful choices are usually SVG (`.svg` extension), PDF (`.pdf`), or PNG (`.png`) if a bitmap format is desired. Alternatively,

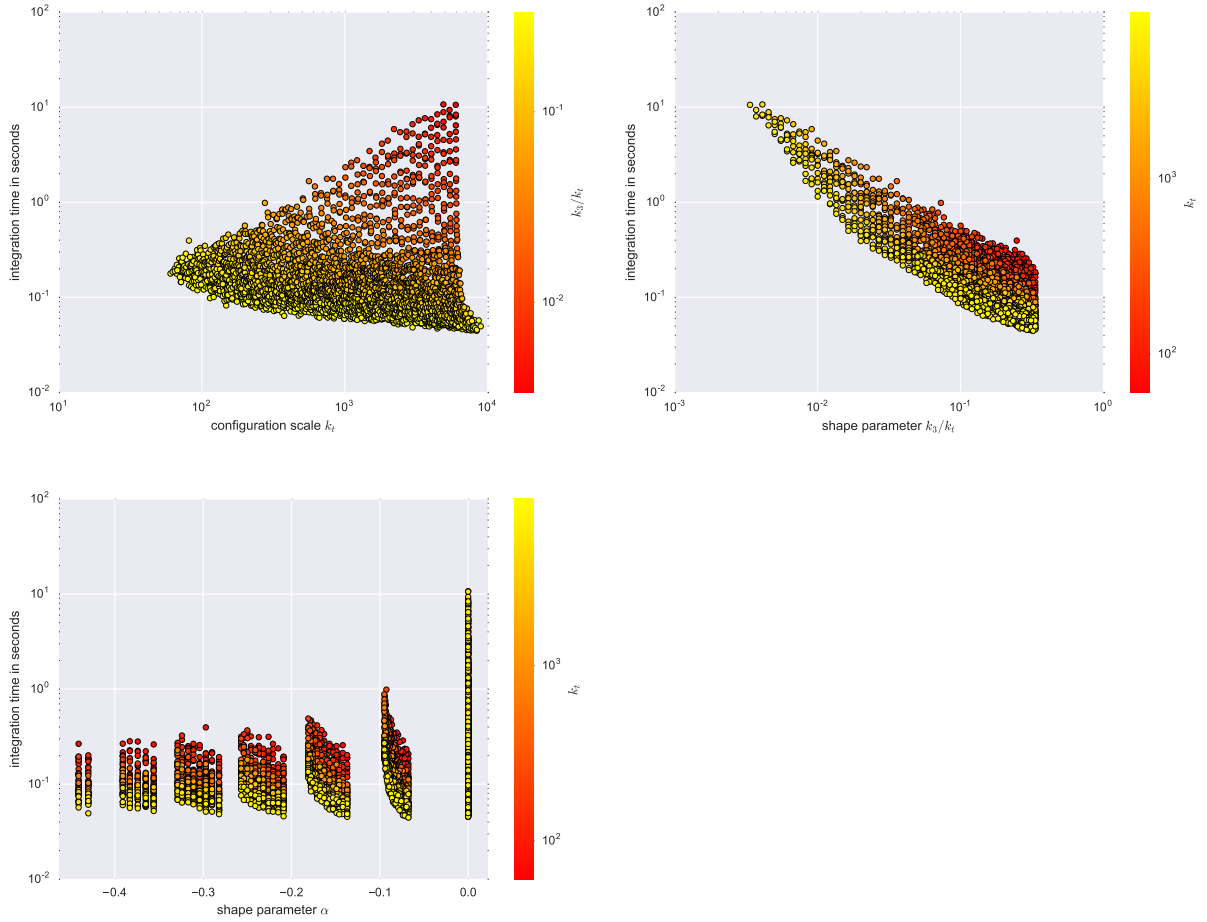


Figure 9. Dependence of integration time on the parameters k_t (top left), $k_3/k_t = (1 - \beta)/2$ (top right) and α (bottom left) in the double quadratic model of §4.3; for definitions, see Eq. (4.1).

specifying a `.py` extension will produce a Python script to generate the Gantt chart, but without executing it. This is useful if further customization is required. For example, by producing a Python script it is possible to manually increase the figure width if the timeline is too compressed for easy reading. An example chart for the `dquad.threepf` task is shown in Fig. 10.

If more detail is required then CppTransport can produce an activity journal in JSON format using the `--journal` command-line argument. It accepts a single parameter that is interpreted as the filename of the output journal. To use the journal for practical analysis it will probably be necessary to write a custom code that parses each record and generates a suitable output.

Avoiding stalls.—CppTransport makes default choices that usually prevent significant stalls. Stalls are more likely in the following circumstances:

- if the repository is located on a slow filing system. Besides allocating work to each worker process, the master process is responsible for aggregating their results into the

main data container `data.sqlite`. The time taken for each aggregation is dominated by the time required for a bulk `INSERT` of rows from each temporary container into the main database.

Depending how many configurations are being computed, and how many time sample points are being retained, the main database may become very large. `CppTransport` has been optimized so that `INSERT` performance is roughly independent of the database size, but its performance may begin to degrade if the database becomes extremely large (bigger than several tens of Gb). On a fast internal SSD `CppTransport` typically achieves $\sim 2 \times 10^5$ `INSERT` s per second. On a conventional hard disc, either internal or attached via a fast interface such as USB or Thunderbolt, it achieves $\sim 5 \times 10^4$ `INSERT` s per second. Network filing systems are often somewhat slower. If you are forced into this situation then it is preferable to use the fastest available disk (eg. a Lustre-type system rather than NFS) in order to prevent aggregations from becoming too slow.

With a slower filing system it can be a good strategy to set a checkpoint interval (or adjust the cache capacity) so that aggregations are distributed over the lifetime of the job. This means that master can be carrying out productive activity while the workers are busy with calculations. The downside of this approach is that a worker may finish its current allocation while the master is performing aggregation. If this will happens it will stall until the master is free to allocate new work.

To mitigate this effect, `CppTransport` monitors how long is spent performing aggregations and adjusts the amount of work it offers to each worker. Initially it will attempt to allocate 60s of work, but if aggregations are taking a long time it will try to allocate *up to* ten times the current mean aggregation time. This reduces the probability that a worker will finish its current allocation while the master is performing aggregation.¹² However, conversely, it increases the risk that the allocation becomes unbalanced in the sense that some workers run out of work items while other workers still have a long queue.

Alternative strategies. Aggregation times are typically not long enough to be problematic. When writing to a hard disk `CppTransport` can typically aggregate a ~ 5 Gb main database in just a few minutes. Problems are likely to occur only in extreme scenarios, where a database grows to many tens of Gb while simultaneously being used over NFS.

- if a large number of workers are used with a slow filing system. Using many workers will generate a large number of aggregation requests, and if the filing system is too slow these can overwhelm the master process. There are possible mitigations:
 - if you are not using a network filing system, ensure that you are not passing the command-line option `--network-mode`. If used this disables SQLite’s write-ahead log mode that confers a significant performance advantage.
 - ensure that you are not defining the `CPPTRANSPORT_STRICT_CONSISTENCY` macro during compilation. If used, this roughly doubles aggregation times. See §4.8.2.

¹²In practice it may allocate less work in order to balance the number of work items assigned to each worker process.

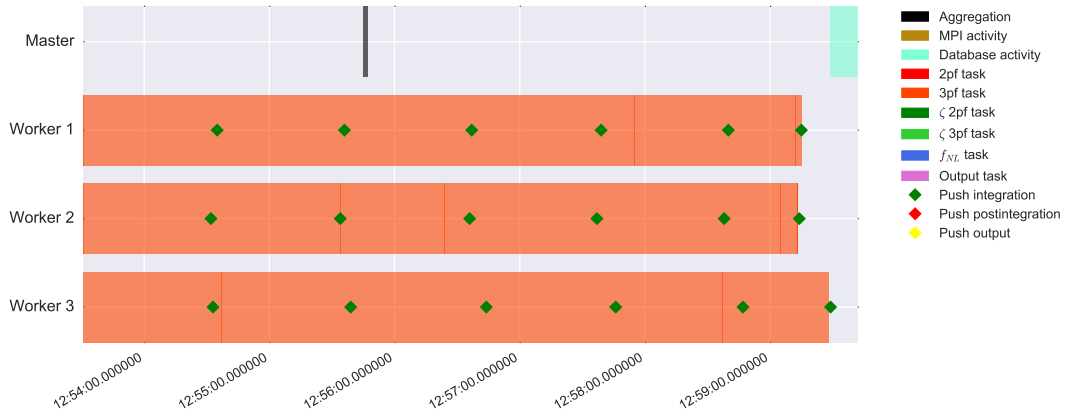


Figure 10. Gantt chart generated by CppTransport’s `--gantt` option, showing worker activity for the task `dqquad.threepf` and `--checkpoint 1`. The diamonds indicate where each worker flushed its cache to a temporary database. Dark grey bars on the master timeline show where the master process was aggregating temporary databases. (In many cases the time spent aggregating was too short to register on the plot. This test was performed on a machine with an SSD; on a machine with a hard disk, aggregation times are usually a few times longer.) The aquamarine bar on the far right-hand side shows database activity associated with checking integrity and performing routine maintenance.

- experiment with different buffer sizes or checkpoint intervals, which will change how aggregation events are distributed over the lifetime of the job. In some scenarios it is faster to perform a small number of large aggregations near the end. In other scenarios it can be faster to perform frequent aggregations throughout the job, because this makes use of time when the master process would otherwise be idle.

4.8 Using the SQLite data container

In §§6–7 we will consider post-integration tasks and show how they can be used to generate observables from the raw n -point functions produced by an integration task. In many cases the facilities offered by these tasks will be quite adequate to carry out a standard analysis of an inflationary model. However, in some circumstances, a nonstandard observable may be needed. In this case it is necessary to extract data for the raw n -point functions. Another reason for needing this data is simply that you may wish to produce your own customized plots.

4.8.1 Table definitions

This data can be retrieved from the main SQLite container `data.sqlite` associated with each content group. As explained above, this is done using SQL queries—yielding a powerful method to easily extract appropriate subsets of the data, formatted in any convenient way.

The SQLite container for any integration task contains the following tables and columns:

1. `time_samples` — contains the list of time sample points.

<code>serial</code>	unique serial number for this sample point
<code>time</code>	numerical value of time, measured in N , using the user-defined conventions established by the initial conditions package.

2. `twopf_samples` — contains the list of sample points for the 2-point function

<code>serial</code>	unique serial number for this sample configuration
<code>conventional</code>	conventionally-normalized wavenumber k corresponding to this configuration
<code>comoving</code>	comoving-normalized wavenumber k corresponding to this configuration
<code>t_exit</code>	time of horizon exit for this wavenumber in the sense $k = aH$
<code>t_massless</code>	mass-point for this wavenumber in the sense $(k/a)^2 = M^2$, where M^2 is the largest eigenvalue of the mass matrix

3. `backg` — contains the time evolution of the background fields

<code>unique_id</code>	unique identifier labelling this row
<code>tserial</code>	reference to serial number <code>time_samples.serial</code> identifying the time sample point for this row
<code>page</code>	the value of each background field is stored in the column <code>coordN</code> , where N is a 0-based integer labelling the fields in the same order that they were declared in the model description file. However, SQLite allows only a limited number of columns per table. To accommodate this CppTransport will store the roughly the first 2000 entries with <code>page</code> equal to 0 and then start a new row with <code>page</code> equal to 1, and so on. The same strategy is used for all data tables
<code>coordN ...</code>	values of the background fields in the order declared in the model description file. All fields come first as a block, followed by their N derivatives as a second block.

4. `twopf_re` — contains real part of field-space 2-point function

<code>unique_id</code>	unique identifier labelling this row. Not used unless strict data consistency checks are enabled by defining the macro <code>CPPTRANSPORT_STRICT_CONSISTENCY</code> during compilation. See §4.8.2.
<code>tserial</code>	reference to serial number <code>time_samples.serial</code> identifying the time sample point for this row
<code>kserial</code>	reference to serial number <code>twopf_samples.serial</code> identifying the wavenumber sample point for this row
<code>page</code>	page number, defined as for <code>backg.page</code> ; see <code>eleN</code> below
<code>eleN ...</code>	

dimensionless components of the real part of the field-space 2-point function, packed in a ‘right-most’ ordering defined as follows. Set $\langle \delta X^a(\mathbf{k}_1) \delta X^b(\mathbf{k}_2) \rangle = (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2) \Sigma^{ab}$, where a, b range over the fields and their canonical momenta (which for the purposes of the 2-point function are the same as the derivatives with respect to N). Then $N = D \times \#a + \#b$, if D is the dimension of phase space (two times the number of fields) and $\#$ is the map that assigns a numerical value to a species in following order: fields first, in the order defined in the model description file, followed by momenta, in the same order as the fields.

The quantity stored is $\text{Re}(k^3 \Sigma^{ab})$, where $k = |\mathbf{k}_1| = |\mathbf{k}_2|$ is the common magnitude of the momenta. This is independent of the comoving normalization, making the results easy to remap into whatever units are convenient.

5. `tensor_twopf` — contains the tensor 2-point function

<code>unique_id</code>	unique identifier labelling this row. Not used unless strict data consistency checks are enabled by defining the macro <code>CPPTRANSPORT_STRICT_CONSISTENCY</code> during compilation. See §4.8.2.
<code>tserial</code>	reference to serial number <code>time_samples.serial</code> identifying the time sample point for this row
<code>kserial</code>	reference to serial number <code>twopf_samples.serial</code> identifying the wavenumber sample point for this row
<code>page</code>	page number, defined as for <code>backg.page</code> ; see <code>eleN</code> below
<code>eleN ...</code>	

dimensionless components of the real part of the tensor two-point function for an individual helicity state γ_s (where $s = +, \times$) and their derivatives $\pi_s = d\gamma_s/dN$, in the following order: $N = 0$ is $\gamma_s \gamma_s$, $N = 1$ is $\gamma_s \pi_s$, $N = 2$ is $\pi_s \gamma_s$ and $N = 3$ is $\pi_s \pi_s$.

If $\langle \gamma_s(\mathbf{k}_1) \gamma_{s'}(\mathbf{k}_2) \rangle = (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2) \Sigma_{ss'}$, where s and s' label helicities, then the quantity stored is $\text{Re}(k^3 \Sigma_{ss'})$.

6. `integration_statistics` — contains integration metadata

<code>kserial</code>	reference to serial number <code>twopf_samples.serial</code> or <code>threepf_samples.serial</code> (depending whether the data is for a 2pf or 3pf task) to which this row corresponds
<code>workgroup</code>	workgroup number for the worker that processed this configuration
<code>worker</code>	worker number for the worker that processed this configuration
<code>integration_time</code>	time required to perform integration, in nanoseconds
<code>batch_time</code>	time required to transfer the integration data into storage, in nanoseconds
<code>steps</code>	number of steps taken by the integrator. Can be used to check whether the integrator is performing an excessive amount of work, which normally indicates that a different algorithm might give better performance
<code>refinements</code>	number of times the density of the time-sample mesh needed to be increased. Not used in the current version of CppTransport.

In addition, tasks sampling the 3-point function include the following extra tables:

7. `threepf_samples` — contains the list of sample points for the 3-point function

<code>serial</code>	unique serial number for this sample configuration
<code>wavenumber1</code>	reference to <code>twopf_samples.serial</code> identifying the k_1 mode for this configuration
<code>wavenumber2</code>	reference to <code>twopf_samples.serial</code> identifying the k_2 mode for this configuration
<code>wavenumber3</code>	reference to <code>twopf_samples.serial</code> identifying the k_3 mode for this configuration
<code>kt_conventional</code>	conventionally-normalized value of k_t for this configuration
<code>kt_comoving</code>	comoving-normalized value of k_t for this configuration
<code>alpha</code>	value of α for this configuration
<code>beta</code>	value of β for this configuration
<code>t_exit_kt</code>	horizon-exit time for this configuration, in the sense $k_t/3 = aH$
<code>t_massless</code>	massless point for this configuration, given by the earliest of the massless points for k_1, k_2, k_3
8. `twopf_im` — contains the imaginary part of the field-space 2-point function
The schema and storage conventions for this table are the same as for the real part of the 2-point function, `twopf_re`.

9. `threepf_momentum`
`threepf_deriv` — contains the real part of the field-space 3-point function
These tables share the same schema. The difference is that `threepf_momentum` stores correlation functions defined using the canonical momenta (rescaled by a^3), whereas `threepf_deriv` stores correlation functions defined using derivatives with respect to N . These have a nontrivial relationship that is not easy to reconstruct without access to model-dependent information, and specifically the A , B and C tensors defined by Dias et al. []. To mitigate difficulties with reconstructing one or other of these sets of correlation functions CppTransport stores both, at the expense of roughly doubling the storage requirements for each 3-point function task.

If the correlation functions produced by CppTransport are to be used as input for a separate-universe type calculation, or are to be compared with the corresponding *outputs*, then it is the

correlation functions involving derivatives that are required.

<code>unique_id</code>	unique identifier labelling this row. Not used unless strict data consistency checks are enabled by defining the macro <code>CPPTRANSPORT_STRICT_CONSISTENCY</code> during compilation. See §4.8.2.
<code>tserial</code>	reference to serial number <code>time_samples.serial</code> identifying the time sample point for this row
<code>kserial</code>	reference to serial number <code>twopf_samples.serial</code> identifying the wavenumber sample point for this row
<code>page</code>	page number, defined as for <code>backg.page</code> ; see <code>eleN</code> below
<code>eleN ...</code>	dimensionless components of the real part of the field-space 3-point function, packed in a ‘right-most’ ordering as for the 2-point function. That is, if $\langle \delta X^a(\mathbf{k}_1) \delta X^b(\mathbf{k}_2) X^c(\mathbf{k}_3) \rangle = (2\pi)^3 \delta(\sum_i \mathbf{k}_i) \alpha^{abc}$, then $N = D^2 \times \#a + D \times \#b + \#c$. The quantity stored is the <i>shape function</i> $\text{Re}(k_1^2 k_2^2 k_3^2 \alpha^{abc})$. As for the other data tables, this object is independent of the comoving normalization and can be easily remapped into any choice of wavenumber normalization.

4.8.2 Strict consistency checking

In rare circumstances it may be useful to enforce strict consistency checks within the database. These checks ensure that there is only entry for each time- and wavenumber-configuration combination, and also ensure that the serial numbers recorded in each data table (such as `backg`, `twopf_re` and so on) refer to valid entries in the sample tables `time_samples`, `twopf_samples` and `threepf_samples`. The price paid for such checks is substantially reduced `INSERT` performance during aggregation, by at least a factor of two but sometimes more.

To enable strict database checks, edit the main header file `transport.h` to define the macro `CPPTRANSPORT_STRICT_CONSISTENCY`, or define it by hand before including any `CppTransport` headers. When enabled, this forces `CppTransport` to use the `unique_id` fields in each data table. These contain a unique integer encoding the time-sample, wavenumber-sample and page number for the row. The extra time cost arises because for each `INSERT` SQLite must check the existing database to ensure there are no conflicts. In a worst-case scenario this means that `INSERT` performance could degrade in proportion to the size of the main database, although typically this is not realized because `CppTransport` takes special measures to avoid it. Nevertheless, if these checks are performed then *some* degradation must be expected as the size of the database grows.

Normally it is best to leave strict checks disabled unless you need them for some special purpose. For example, this situation might arise if you want uniqueness to be enforced via `PRIMARY KEY` constraints after the database has been constructed; SQLite does not allow primary keys to be added later. Alternatively you could consider post-processing the database to add your own unique identifiers and creating a `UNIQUE` index.

5 Options for integration tasks

5.1 General options

This section documents the options that can be used when customizing integration tasks. Typically options are set using member functions provided by each task object, such as the

`twopf_task` and `threepf_cubic_task` objects used in §4.3.

- `set_name(std::string)`
Sets the task name to the supplied string
- `set_description(std::string)`
Sets an (optional) description field. Reports for this task (either obtained at the command line by the `--info` switch, or using the HTML report generator) include this description field where it is present.
- `bool get_adaptive_ics()`
`set_adaptive_ics(bool)`
Get or set the current adaptive initial conditions state.

`CppTransport` sets initial conditions for each n -point function by working in the universal, massless approximation. This will be valid provided the initial time is set substantially earlier than the massless point for each wavenumber participating in the correlation function, as defined on p.48 in §4.4.2. The massless time is not later than the horizon exit time for the corresponding wavenumber, but can be earlier if there is a massive mode in the spectrum.

Generally, increasing the number of e-folds of massless evolution will improve `CppTransport`'s estimate of the correlation functions at horizon exit. The accuracy of these estimates is the principal factor determining accuracy of the evolution in the super-horizon regime. Unfortunately, subhorizon evolution is very expensive. In this phase the individual wavefunctions oscillate with exponentially increasing frequency as we move deeper into the subhorizon epoch. The correlation functions themselves do not oscillate, and therefore to ensure accuracy the stepper must adjust its step size so that counterbalancing oscillatory contributions cancel to an acceptable precision. The maximum acceptable step size decreases rapidly on subhorizon scales.

In normal circumstances this means we wish to have just enough e-folds of massless evolution, but not more. Usually it is sufficient to have between 3 and 5 e-folds of massless evolution, with 4 a good default choice. To make this possible `CppTransport` supports two ways to set initial conditions for each n -point function—*uniform* and *adaptive*. With uniform initial conditions `CppTransport` will compute an initial condition for each n -point function at the initial time specified in the initial conditions package (§4.3) and evolve it from there. The advantage is that each correlation function gets the same initial time, so it is possible to compare their values at any subsequent point. The disadvantage is that this initial time may give some n -point functions a very large number of e-folds of massless evolution. Often this makes the corresponding integrations impractically expensive.

The alternative is adaptive initial conditions. Using adaptive initial conditions, `CppTransport` will compute a customized initial condition a fixed number of e-folds before the massless point for the correlation function in question. (As explained on p.66, the massless point for a bispectrum configuration is defined to be the earliest massless point among all participating wavenumbers.) This choice is often dramatically faster than using uniform initial conditions. In many cases it is the only feasible way to perform

the calculation. The disadvantage is that not all correlation functions will have sample data available at early times, because sampling begins at different times for different configurations. `CppTransport` will only keep sample points for which all configurations have data available.

Adaptive initial conditions are the recommended setting for all `CppTransport` tasks. However, because they impose more stringent requirements on the initial conditions they are not enabled by default. This can be done by passing the value `true` to `set_adaptive_ics()`, in which case the number of massless e-folds will default to 4, or by calling `set_adaptive_ics_efolds()` with an alternative value.

If the initial time specified as part of the initial conditions package does not allow this number of e-folds prior to the earliest massless point, then the task will throw a `transport::runtime_exception` exception.

- `double get_adaptive_ics_efolds()`
`set_adaptive_ics_efolds(double N)`

Get or set the number of e-folds of massless evolution used by adaptive initial conditions.

- `double get_astar_normalization()`
`set_astar_normalization(double)`

For concrete calculations `CppTransport` must convert conventionally-normalized wavenumbers to comoving-normalized ones. This involves a choice of scale factor a_* at the distinguished time N_* when the conventionally-normalized scale $k = 1$ leaves the horizon.

Normally it is not necessary to be aware of what choice is made for a_* , because as explained in §4.8 the database stores *dimensionless* correlation functions. The normalization of these correlation functions does not depend on a_* and therefore they are simple to remap into whatever wavenumber normalization is convenient for the problem at hand.

By default `CppTransport` sets $a_* = \exp(0) = 1$. The current implementation of the transport integrator uses dimensionless correlation functions, and therefore the numerical solutions are independent of its value. As a result this setting can mostly be ignored, unless you want a specific normalization for the purpose of producing plots or tables.

- `bool get_collect_initial_conditions()`
`set_collect_initial_conditions(bool)`

Get or set the current collection state for initial conditions.

To assist comparison of the results produced by `CppTransport` with other methods of computing n -point functions, it is possible to have `CppTransport` write extra table into the SQLite container that gives the field-values at horizon exit for each configuration. For tasks computing the 2-point function only, `CppTransport` will write a table called `horizon_exit_values` that records the field values at horizon exit for the corresponding wavenumber. For tasks computing the 3-point function `CppTransport` writes two tables: for each configuration, `horizon_exit_values` records field values at horizon-exit for the

wavenumber which exits earliest. In addition `kt_horizon_exit_values` contains the field values at horizon-exit for the average scale $k_t/3$.

Note that these are *not* the initial conditions used by CppTransport internally.

- `boost::optional<unsigned int> get_default_checkpoint()`
`set_default_checkpoint(unsigned int)`
`unset_default_checkpoint()`

Get or set the current default checkpoint interval.

A default checkpoint interval can be set on a per-task basis. If no `--checkpoint` switch is given on the command line then the default checkpoint interval is applied, otherwise the value supplied to `--checkpoint` is used. The current checkpoint interval can be cleared using `unset_default_checkpoint()`.

If there is no currently-set default interval then `get_default_checkpoint()` returns an empty `boost::optional` (see [here](#)). Otherwise, it returns a `boost::optional` containing the current checkpoint interval in minutes.

5.2 Two-point function tasks

Two-point function tasks need few specific options, and those that exist are supplied through the constructor. Its general form is

```
twopf_task(
    std::string name,
    initial_conditions ics,
    range time_samples,
    range k_samples,
    bool adaptive_ics=false
)
```

This constructs a task with the given name and initial conditions, and the specified time- and wavenumber sample points. The `range` objects can be instances of either `basic_range` or `aggregate_range` (§4.3). If the boolean `adaptive_ics` is supplied then it determines whether adaptive initial conditions are automatically enabled. If `true` the task will default to using 4 massless e-folds, but this can be changed by calling `set_adaptive_ics_efolds()`.

5.3 Three-point function tasks

CppTransport provides two different interfaces for specifying three-point function tasks. The differences relate to the way in which the sample configurations are specified.

5.3.1 Cubic (k_1, k_2, k_3) mesh

One possibility is to build a set of bispectrum configurations from the Cartesian product $k_s \times k_s \times k_s$ built out of some range of wavenumbers `ks`. This option was used to build the task `dquad.threepf` used as an example in §4.

To generate a task in this way one should use the `threepf_cubic_task` constructor. Its signature is

```

threepf_cubic_task(
    std::string name,
    initial_conditions ics,
    range time_samples,
    range ks,
    bool adaptive_ics=false,
    StoragePolicy storage_policy = DefaultStoragePolicy,
    TrianglePolicy triangle_policy = DefaultTrianglePolicy
)

```

The last three parameters are optional, and if omitted their default values will be used. The range `ks` is used to construct a Cartesian mesh of wavenumbers as explained above, and the remaining parameters share their meaning with the constructor for two-point function tasks described in §5.2. For details of the `StoragePolicy` and `TrianglePolicy` concepts see §5.3.3 and §5.3.4 respectively.

There is no need to specify a set of wavenumbers at which to sample the 2-point function. Samples will automatically be recorded at points corresponding to each wavenumber appearing on an external leg of the 3-point function. In this case that means the 2-point function will be sampled at the wavenumbers in `ks`.

5.3.2 Fergusson–Shellard (k_t, α, β) mesh

Sampling from a wavenumber cube `ks`³ is convenient for some purposes but awkward for others. In particular, if the intention is to sample a series of wavenumber configurations probing the squeezed limit of the bispectrum then there may be more efficient ways to proceed. A good choice is to work with parameters that directly specify the configuration shape. For this purpose `CppTransport` uses the (α, β) parameters introduced by Fergusson & Shellard [53]; see Eq. (4.1).

To build a task from a grid of k_t , α and β combinations one should use the `threepf_alphabeta_task` constructor:

```

threepf_alphabeta_task(
    std::string name,
    initial_conditions ics,
    range time_samples,
    range kts,
    range alpha,
    range betas,
    bool adaptive_ics=false,
    StoragePolicy storage_policy = DefaultStoragePolicy,
    TrianglePolicy triangle_policy = DefaultTrianglePolicy
)

```

As for `threepf_cubic_task` the last three parameters are optional. The sample configurations are built from restricting the Cartesian product of the (k_t, α, β) parameters `kts` \times `alphas` \times `betas` to valid triangle configurations.

As for cubic tasks, the sample points for the 2-point function are not specified separately. `CppTransport` will compute the wavenumbers appearing on each external leg of the 3-point function and use these to build a list of sample points for the 2-point function. For tasks specified using combinations of (k_t, α, β) this means that the sample points can be irregularly spaced if the sampled set of bispectrum configurations is sparse.

5.3.3 Specifying a storage policy

Sometimes the grids `ks × ks × ks` or `kts × alphas × betas` will include combinations that are not needed for the task at hand. Rather than wastefully compute these, `CppTransport` allows them to be omitted by specifying a *storage policy*.

If supplied, a storage policy should be an instance of a callable object that accepts a reference to a `transport::threepf_kconfig` object and returns a valid `transport::storage_outcome`:

```
transport::storage_outcome (StoragePolicy)(const transport::threepf_kconfig& config)
```

The `transport::threepf_kconfig` data structure specifies the configuration that is to be inspected. Its fields are public data members:

- `serial`
The proposed unique serial number for this configuration.
- `k1_serial`, `k2_serial`, `k3_serial`
The serial numbers for the wavenumbers k_1 , k_2 , k_3 associated with each external leg.
- `k1_conventional`, `k2_conventional`, `k3_conventional`
The conventionally-normalized wavenumbers associated with each external leg.
- `k1_comoving`, `k1_comoving`, `k3_comoving`
The comoving-normalized wavenumbers associated with each external leg.
- `kt_conventional`, `kt_comoving`
The conventional- and comoving-normalized k_t associated with this configuration.
- `alpha`, `beta`
The α and β values associated with this configuration.

The configuration presented for inspection is guaranteed to be a valid triangle as determined by the active `TrianglePolicy` (§5.3.4). The callable should inspect the and determine whether it should be accepted or rejected. The default storage policy will accept all configurations.

To accept this configuration the policy should return `transport::storage_outcome::accept`. To reject, it should return either:

- `transport::storage_outcome::reject_remove`
When constructing this configuration, it may have been necessary to assign unique serial numbers to new configurations for the two-point function. This will happen if at least one leg of the bispectrum corresponds to a wavenumber that has not yet been allocated a unique number.
If `reject_remove` is specified then `CppTransport` will reject the configuration and deallocate any serial numbers that were speculatively assigned to ‘new’ two-point function configurations.
- `transport::storage_outcome::reject_retain`
Alternatively, `reject_retain` allows these serial numbers to be retained.

A typical use case for this functionality occurs when you wish to subsample a cubic grid. Suppose the range `ks` contains a set $\{k_1, k_2, \dots, k_m\}$ of wavenumbers, ordered

so that $k_i < k_j$ if $i < j$. Therefore k_m corresponds to the shortest physical scale that will be sampled. The set of isosceles triangles containing this mode is given by the configurations (k_m, k_i, k_i) for all i , and a suitable storage policy picking out this subset might be

```

1  struct StoragePolicy
2  {
3      transport::storage_outcome operator()(const transport::threepf_kconfig& data)
4      {
5          if(data.k1_serial == m) return(transport::storage_outcome::accept);
6          else return(transport::storage_outcome::reject_retain);
7      }
8  };

```

Each configuration will be presented to `StoragePolicy` for inspection in the order determined by the Cartesian product `ks`³, so by returning `reject_retain` we can ensure that the serial numbers assigned to the 2-point function configurations will match the ordering in `ks`.

5.3.4 Specifying a triangle policy

`CppTransport` also allows specification of a *triangle policy*. This is used to determine which members of the grids `ks` \times `ks` \times `ks` and `kts` \times `alphas` \times `betas` are considered valid triangles.

`CppTransport`'s default triangle policy imposes two conditions: first, it requires $k_1 + k_2 + k_3 \geq 2 \max\{k_1, k_2, k_3\}$. This is the geometrical condition that the sides $\{k_1, k_2, k_3\}$ can form a triangle and is equivalent to demanding that the sum of the two shortest sides is longer than the longest side. If this is not satisfied then the 'triangle' cannot be closed.

Second, it imposes the condition $k_1 \geq k_2 \geq k_3$. This is intended to prevent unnecessary repeat calculations. If we are interested only in connected correlation functions then we are free to reorder the fields inside any equal-time correlation function $\langle \delta X^a(\mathbf{k}_1) \delta X^b(\mathbf{k}_2) X^c(\mathbf{k}_3) \rangle$ because the failure of any pair of X s to commute will produce contact terms. Because `CppTransport` solves the correlation functions for all index combinations (a, b, c) , this reordering property implies that it is only necessary to compute those configurations satisfying $k_1 \geq k_2 \geq k_3$. The remaining configurations can be determined by permuting the index labels.

For some purposes, however, it is convenient to drop this restriction or to adopt a different ordering. One use case is to produce bispectrum shape plots in the (α, β) plane. The restriction $k_1 \geq k_2 \geq k_3$ implies that `CppTransport` will produce correlation functions that cover only $1/3! = 1/6$ of the allowed (α, β) space, and in principle the remaining regions can be determined by suitable transformations of the region that is computed. However, this transformation will map a rectangular mesh in the computed region to a non-rectangular mesh in the other regions. Many plotting libraries require a uniform rectangular mesh of points in order to produce surface or 3-dimensional plots, making these non-rectangular transformed meshes unacceptable. In this case, instead of splining the transformed regions and resampling them on a rectangular mesh, it can be simpler to absorb the factor of 6 computation cost and have `CppTransport` compute these points directly.

A triangle policy is an instance of a callable object that determines whether a given configuration forms a triangle. The ‘cubic’ and ‘ $\alpha\beta$ ’ constructors require different types of policy:

- for a ‘cubic’ constructor, the triangle policy should accept 6 arguments and return a `bool` indicating whether the configuration is valid:

```
bool (TrianglePolicy)(unsigned i, unsigned j, unsigned k, double k1, double k2, double k3)
```

The arguments `i`, `j`, `k` refer to the index of the k_1 , k_2 , k_3 values (respectively) within the original range `ks`. The arguments `k1`, `k2`, `k3` give these (conventionally-normalized) wavenumber values directly.

The default `CppTransport` policy rejects triangles according to the following criteria:¹³

```
1 // impose ordering k1 > k2 > k3
2 if(i < j) return false;
3 if(j < k) return false;
4
5 // impose triangle
6 double max = std::max(std::max(k1, k2), k3);
7 return(k1 + k2 + k3 - 2.0*max >= 0.0);
```

- for an ‘ $\alpha\beta$ ’ task, the triangle policy should accept just two arguments corresponding to the values of α and β ,

```
bool (TrianglePolicy)(double alpha, double beta)
```

The default policy rejects triangles as follows:

```
1 // beta should lie between 0 and 1
2 if(beta < 0.0) return false;
3 if(beta > 1.0) return false;
4
5 // alpha should lie between 1-beta and beta-1
6 if(beta - 1.0 - alpha > 0.0) return false;
7 if(alpha - (1.0 - beta) > 0.0) return false;
8
9 // impose k1 > k2 > k3
10 if(alpha < 0) return false;
11 if(beta - (1.0 + alpha)/3.0 < 0.0) return false;
```

In addition, it requires that none of the ‘squeezing’ measures $1 - \beta$, $|1 + \alpha - \beta|$ and $|1 - \alpha + \beta|$ becomes too small. By default the cutoff is taken to be 10^{-8} .

6 Adding postintegration tasks

Although integration tasks are always the first step in using `CppTransport`, for most purposes the n -point functions they produce need to be reprocessed into observables. At a minimum we normally require predictions for the correlation functions of the primordial curvature

¹³In reality the policies do not perform literal `<` or `>` comparisons because of possible issues with floating point arithmetic. These subtleties are ignored here, and the policy is presented as if it were implemented purely using its mathematical definition. The same applies to the default policy for ‘ $\alpha\beta$ ’ tasks.

perturbation ζ . It is ζ that eventually determines the statistics of the observed density perturbation—although it may happen (where an adiabatic limit is not achieved by the end of inflation) that these observable statistics also depend on post-inflationary physics that is not handled by CppTransport. In such cases the ζ correlation functions produced by the CppTransport platform should be used as initial conditions for a Boltzmann solver (or equivalent) that is capable of following their evolution through the subsequent radiation- and matter-dominated phases.

6.1 ζ tasks for the two- and three-point functions

Post-processing or ‘postintegration’ tasks accept output from integration tasks (or other postintegration tasks) and convert it into some other form. To produce ζ correlation functions we need to specify post-processing tasks that can perform the gauge transformation from field space into ζ .

Returning to the example of double-quadratic inflation, we can ‘connect’ suitable two- and three-point function tasks for ζ to the existing integration tasks `tk2` and `tk3`. It is only necessary to add the following lines at the end of the `write_tasks()` function:

```

1 transport::zeta_twopf_task<> ztk2("dquad.twopf-zeta", tk2);
2 ztk2.set_description("Convert the output from dquad.twopf into a zeta 2-point function");
3
4 transport::zeta_threepf_task<> ztk3("dquad.threepf-zeta", tk3);
5 ztk3.set_description("Convert the output from dquad.threepf into zeta 2- and 3-point functions");
6
7 repo.commit(ztk2);
8 repo.commit(ztk3);

```

The constructor for `zeta_twopf_task` accepts a name and an instance of a `twopf_task`, whereas the constructor for `zeta_threepf_task` accepts a name and an instance of a generic `threepf_task`. The 3-point function task may have been constructed using either `threepf_cubic_task` or `threepf_alphabeta_task`. It is not possible to use a `twopf_task` with `zeta_threepf_task` or a `threepf_task` with `zeta_twopf_task`.

After constructing `ztk2` and `ztk3` they are committed to the repository database using `repo.commit()`, as for any repository object. The original `commit()` calls for `tk2` and `tk3` can be removed because CppTransport will realize that these integration tasks must be stored in the repository database in order for `ztk2` and `ztk3` to make sense.

Build the `dquad` executable as before and invoke it with an instruction to execute the new `dquad.threepf-zeta` task:

```

1 mpiexec -n 4 dquad -v -r test-zeta --create --task dquad.threepf-zeta

```

As usual, the `-n` argument of `mpiexec` should be adjusted to use a suitable number of processes on your machine. CppTransport will print short updates as it carries out each task:

```

Task manager: processing task 'dquad.threepf' (1 of 2)
Committed content group '20160516T130625' for task 'dquad.threepf' at 2016-May-16 14:12:44
Task manager: processing task 'dquad.threepf-zeta' (2 of 2)
Committed content group '20160516T131244' for task 'dquad.threepf-zeta' at 2016-May-16 14:13:50
Task manager: processed 2 database tasks in wallclock time 7m 24.5s | time now 2016-May-16 14:13:50

```

Although we only asked for the `dquad.threepf-zeta` task, CppTransport has scheduled execution of both `dquad.threepf` and `dquad.threepf-zeta`. This happens because it is aware

that `dquad.threepf-zeta` needs content from `dquad.threepf` before it can be processed. If no content groups are available for `dquad.threepf` then it is added to the list of tasks to be processed. The same applies for any chain of dependent tasks; if a task specified on the command line depends on output from some other task for which no content groups are available, CppTransport will automatically schedule execution of these tasks.

If we now re-run the same command (removing the unnecessary option `--create`), CppTransport will notice that content for `dquad.threepf` is already available and assume that it should be used to feed the new execution of `dquad.threepf-zeta`:

```
1 $ mpiexec -n 4 dquad -v -r test-zeta --create --task dquad.threepf-zeta
2 Committed content group '20160516T131956' for task 'dquad.threepf-zeta' at 2016-May-16 14:21:02
3 Task manager: processed 1 database task in wallclock time 1m 6.97s | time now 2016-May-16
  ↪ 14:21:02
```

Checking the number of content groups attached to each task using `--status` shows that `dquad.threepf-zeta` now has 2 groups, while `dquad.threepf` has only one:

```
1 $ ./dquad -r test-zeta/ --status
2 Available tasks:
3 Task                Type                Last activity  Outputs
4 dquad.threepf       integration         2016-May-16 13:12:44    1
5 dquad.threepf-zeta postintegration     2016-May-16 13:21:02    2
6 dquad.twopf         integration         2016-May-16 13:06:25    0
7 dquad.twopf-zeta   postintegration     2016-May-16 13:06:25    0
```

6.2 Applying tags to control which content groups are used

When several suitable content groups are available to feed into a postintegration task, CppTransport must decide which one should be used. By default it will use the most recently-generated group, but this not always the appropriate choice. For example, we might have several content groups attached to the task `dquad.threepf`, perhaps generated using different steppers or different numerical tolerances. To control which content groups are used by postintegration tasks CppTransport allows *tags* to be attached to each group. These are short, descriptive strings that label some property of the group. (Of course, these labels may be useful in their own right in addition to their ability to control selection of content groups.)

Using the `--tag` switch, tags can be attached to content groups at the time of generation. Alternatively they may be applied later using `--add-tag` (see §8.1.2). For example, suppose we generate two content groups for the same integration task, one using the Dormand–Prince 4th/5th-order stepper and another using the Fehlberg 7th/8th-order stepper. This could be done by compiling two different executables using different model description files, or by editing the model description file and rebuilding. Using `--tag`, we can tag each of these content groups appropriately:

```
1 $ mpiexec -n 4 dquad -v -r test-tags --create --task dquad.threepf --tag stepper-dopri5
2 $ mpiexec -n 4 dquad -v -r test-tags --task dquad.threepf --tag stepper-fehlberg78
```

It can be checked that the tags have been correctly applied by using `--info` with the content group name, or by generating an HTML report and viewing the group records. We could have specified multiple tags, if necessary, by repeating the `--tag` argument for each one. There is no limit to the number of tags that can be applied.

To compare the results from each stepper we need to obtain ζ predictions from each content group by feeding them to `dquad.threepf-zeta`. This can be done by specifying the appropriate tag (or group of tags) when we launch the `dquad.threepf-zeta` job:

```
1 $ mpiexec -n 4 dquad -v -r test-tags --tag stepper-dopri5 --task dquad.threepf-zeta
```

This time, the option `--tag` has two meanings: first, as for an integration task, the resulting content group will be tagged with whatever labels we specify, here ‘`stepper-dopri5`’. Second, when searching for content groups to use as a source, `CppTransport` will restrict attention to those with matching tags. If multiple tags are specified then `CppTransport` will attempt to match them all, and if no suitable content groups are found then the task will fail with an error:¹⁴

```
1 $ mpiexec -n 4 dquad -v -r test-tags --tag no-matching-tag --task dquad.threepf-zeta
2 Repository error: no matching content groups for task 'dquad.threepf'
```

This process can be repeated. For example, in §7 we will see how to build derived products and generate them using output tasks. Each output task draws its data from a collection of integration and postintegration tasks such as `dquad.threepf` and `dquad.threepf-zeta`. By specifying a collection of tags while executing the output task we can cause it to select input data that satisfy specific labels such as `stepper-dopri5` or `stepper-fehlberg78`.

Selecting a content group by name.—Alternatively, it is possible to select a content group by name. To do this, specify the name as a tag. The resulting content groups will themselves be tagged with the original group name, meaning that in principle it is possible to use this feature to follow chains of groups back to an original integration content group. In practice, however, this kind of dependency tracking is best performed using HTML reports. These can generate dependency diagrams that summarize the interrelation between content groups more efficiently than a large number of tags.

The option to specify content groups by name remains useful when it is necessary to force a particular group to be used.

6.3 Paired ζ tasks

It sometimes happens that the output from an integration task is of limited interest by itself. For example, if our interest is to determine the observational viability of a particular inflationary model then we only require predictions for ζ , at least if a suitable adiabatic limit is reached during the inflationary phase. In these circumstances the content group generated by an integration task will be used only for post-processing by other postintegration tasks. This is such a common occurrence that `CppTransport` provides a short-cut enabling a pair of coupled integration/postintegration tasks to be processed simultaneously. Tasks coupled in this way are said to be *paired*.

To pair the postintegration tasks `ztk2` and `ztk3` with their parent integration tasks, use the `set_paired()` method. The C++ code used to generate these tasks could be replaced by

¹⁴If a task has no content groups, but tags are specified on the command line, then `CppTransport` will schedule execution of the corresponding task. The generated content group will be labelled with the given tags. But if content groups *are* present, simply without matching tags, then `CppTransport` will issue an error. The presumption is that tags have been specified with an intention to pick out a content group with specific properties.


```

1  transport::zeta_twopf_task<> ztk2("dquad.twopf-zeta", tk2);
2  ztk2.set_description("Convert the output from dquad.twopf into a zeta 2-point function");
3  ztk2.set_paired(true);
4
5  transport::zeta_threepf_task<> ztk3("dquad.threepf-zeta", tk3);
6  ztk3.set_description("Convert the output from dquad.threepf into zeta 2- and 3-point functions");
7  ztk3.set_paired(true);
8
9  repo.commit(ztk2);
10 repo.commit(ztk3);

```

Once tasks have been paired in this way:

- asking CppTransport to execute the *integration* task will generate a content group for it, as usual. This content group can be used in the same way as any other.
- asking CppTransport to execute the *postintegration* task will commence simultaneous processing of the integration/postintegration pair. The postintegration task will not look for an existing content group attached to the integration task, as described above; a new integration content group is generated every time. To mark that this content group is paired with a postintegration group, CppTransport will add the suffix ‘-paired’ to its name.

Notice that this means it isn’t possible to select a pre-existing content group to use with a paired postintegration task.

During simultaneous processing, the gauge transformation from field-space to ζ will be calculated on-the-fly, without writing all the integration data out to a database and then reading it back again as with unpaired post-processing. This means that paired tasks normally execute more quickly than unpaired tasks.

Task options.—It is possible to specify independent checkpoint intervals for the tasks in an integration/postintegration pair, but in the event of failure the data stored in each container will be synchronized. In practice this means that data in one container that has no counterpart in the other will be discarded, and therefore there is no real use case for unequal checkpoint intervals.

6.4 Using ζ SQLite data containers

§4.8 described the database containers used to hold data products from an integration task. The data products from postintegration tasks are handled very similarly. In particular, each content group will have the same physical layout shown in Fig. 5. All n -point functions and supporting metadata are aggregated into a main container `data.sqlite`, and logs are left in the directory `logs`.

6.4.1 ζ two-point function tasks

The SQLite container for a task generating the ζ two-point function will contain the following tables:

1. `time_samples` — contains the list of time sample points.
This table duplicates, and is inherited from, the one described in §4.8 (see p.64).
2. `twopf_samples` — contains the list of sample points for the 2-point function
This table duplicates, and is inherited from, the one described in §4.8 (see p.64).

3. `zeta_twopf` — contains the real part of the ζ 2-point function

<code>unique_id</code>	unique identifier labelling this row. Not used unless strict data consistency checks are enabled by defining the macro <code>CPPTRANSPORT_STRICT_CONSISTENCY</code> during compilation. See §4.8.2.
<code>tserial</code>	reference to serial number <code>times_samples.serial</code> identifying the time sample point for this row
<code>kserial</code>	reference to serial number <code>twopf_samples.serial</code> identifying the wavenumber sample point for this row
<code>twopf</code>	dimensionless value of the real part of the ζ 2-point function, $\langle \zeta(\mathbf{k}_1)\zeta(\mathbf{k}_3) \rangle = (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2) P_\zeta$. The value stored is $\text{Re}(k^3 P_\zeta)$.

4. `gauge_xfm1` — contains the linear gauge transformation N_a
The required Fourier-space gauge transformation has the form

$$\zeta(\mathbf{k}) = N_a(\mathbf{k})\delta X^a(\mathbf{k}) + \frac{1}{2} \int \frac{d^3q}{(2\pi)^3} \frac{d^3r}{(2\pi)^3} \delta(\mathbf{k} - \mathbf{q} - \mathbf{r}) N_{ab}(\mathbf{q}, \mathbf{r}) \delta X^a(\mathbf{q}) \delta X^b(\mathbf{r}) + \dots, \quad (6.1)$$

where δX^a , δX^b (and so on) label fluctuations over the full phase space of fields and their derivatives with respect to N , and the omitted terms represented by ‘ \dots ’ are higher order X . Expressions for the transformation coefficients N_a and N_{ab} may be extracted from Dias et al. [54]. In the notation of that reference, the expressions used by `CppTransport` correspond to ζ_1^{simple} and ζ_2^{simple} , making N_a independent of \mathbf{k} in practice.

The ζ post-processing tasks write these transformation coefficients into the data containers. Specifically, the table `gauge_xfm1` is associated with production of the ζ power spectrum, for which only N_a is required. Although the expression used for N_a in current versions is momentum independent, `CppTransport` does not assume this will always be the case and records the gauge transformation for each momentum configuration.

<code>unique_id</code>	unique identifier labelling this row. Not used unless strict data consistency checks are enabled by defining the macro <code>CPPTRANSPORT_STRICT_CONSISTENCY</code> during compilation. See §4.8.2.
<code>tserial</code>	reference to serial number <code>times_samples.serial</code> identifying the time sample point for this row
<code>kserial</code>	reference to serial number <code>twopf_samples.serial</code> identifying the wavenumber sample point for this row
<code>page</code>	page number, defined as for <code>backg.page</code> in §4.8; see p.64
<code>elem ...</code>	components of N_a for this momentum configuration, packed with $M = \#a$. Here, as in §4.8, ‘ $\#$ ’ is the map that takes a species label to its numeric equivalent defined by the order of declaration in the model description file. All fields come first, followed by all field derivatives in the same order. Notice that the gauge transformation (6.1) is taken to be written in terms of <i>derivatives</i> , as in Ref. [54], and not canonical momenta. Notice that because ζ is dimensionless but the δX^a have dimensions of mass, N_a has dimensions of inverse mass. It therefore scales with the value assigned to the Planck scale M_{P} .

6.4.2 ζ three-point function tasks

In addition to the generic tables described above, postintegration tasks that generate the ζ three-point function also write the following tables to the data container:

1. `threepf_samples` — contains the list of sample points for the 3-point function. This table duplicates, and is inherited from, the one described in §4.8 (see p.66).

2. `threepf` — contains the real part of the ζ 3-point function

`unique_id` unique identifier labelling this row. Not used unless strict data consistency checks are enabled by defining the macro `CPPTRANSPORT_STRICT_CONSISTENCY` during compilation. See §4.8.2.

`tserial` reference to serial number `times_samples.serial` identifying the time sample point for this row

`kserial` reference to serial number `twopf_samples.serial` identifying the wavenumber sample point for this row

`threepf` **dimensionless value** of the real part of the ζ 3-point function. If this is taken to satisfy $\langle \zeta(\mathbf{k}_1)\zeta(\mathbf{k}_2)\zeta(\mathbf{k}_3) \rangle = (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) B_\zeta$ then the stored quantity is the dimensionless shape function $k_1^2 k_2^2 k_3^2 B_\zeta$.

`redbsp` **dimensionless reduced bispectrum**, defined by

$$\frac{6}{5} f_{\text{NL}}(k_1, k_2, k_3) = \frac{B_\zeta(k_1, k_2, k_3)}{P_\zeta(k_1)P_\zeta(k_2) + P_\zeta(k_1)P_\zeta(k_3) + P_\zeta(k_2)P_\zeta(k_3)}. \quad (6.2)$$

3. `gauge_xfm2_123`

`gauge_xfm2_213`

`gauge_xfm2_312` — contains the quadratic gauge transformation N_{ab}

For each bispectrum configuration there are three possible assignments for N_{ab} . `CppTransport` writes them all to the data container, in three separate tables with the mapping:

`gauge_xfm_123` $N_{ab}(\mathbf{k}_2, \mathbf{k}_3)$

`gauge_xfm_213` $N_{ab}(\mathbf{k}_1, \mathbf{k}_3)$

`gauge_xfm_312` $N_{ab}(\mathbf{k}_1, \mathbf{k}_2)$

The columns in each table are:

`unique_id` unique identifier labelling this row. Not used unless strict data consistency checks are enabled by defining the macro `CPPTRANSPORT_STRICT_CONSISTENCY` during compilation. See §4.8.2.

`tserial` reference to serial number `times_samples.serial` identifying the time sample point for this row

`kserial` reference to serial number `twopf_samples.serial` identifying the wavenumber sample point for this row

`page` page number, defined as for `backg.page` in §4.8; see p.64

`elem ...` components of N_{ab} for this momentum configuration and momentum assignment, packed with the right-most ordering $M = D \times \#a + \#b$. As for the linear gauge transformation, the expressions assume (6.1) is written in terms of derivatives with respect to e-folding N rather than canonical momenta.

On superhorizon scales all the gauge transformation coefficients become independent of momenta.

6.5 Inner-product tasks to compute f_{NL} -like amplitudes

Production of ζ correlation functions is not the only kind of post-processing that could be considered. In principle it is possible to implement `CppTransport` postintegration tasks to compute almost any observable of interest, but at present only one option is offered—an inner product between the numerically-computed bispectrum and one of the standard bispectrum shapes.

To generate such inner products we use an `fNL_task`. `CppTransport` uses this name because, *under certain circumstances*, the amplitudes they produce may be related to the f_{NL} amplitudes reported by surveys of the cosmic microwave background anisotropies or the large-scale galaxy distribution. However, this interpretation should be treated with caution. As will be explained below, there is no necessary relation between these inner products and the quantities observed by some particular instrument, and to obtain truly accurate results requires a more careful calculation. For an example, see Ref. [55].

To compute an inner product we must provide a source of 3-point function data by attaching a `zeta_threepf_task`. However, `CppTransport` places restrictions on the source 3-point functions for which it can compute inner products. In particular:

- currently, inner products are supported only for 3-point function tasks built from a linear grid (whether of cubic or $\alpha\beta$ type).
- the grid should be complete—no configurations should be dropped by the storage policy.

The inner product between two bispectra is defined to be a sum over the corresponding dimensionless shape functions. Given a bispectrum $B(k_1, k_2, k_3)$, its shape function is $S \equiv (k_1 k_2 k_3)^2 B(k_1, k_2, k_3)$ and the inner product between two bispectra B_1, B_2 satisfies [56, 57]

$$\langle\langle B_1, B_2 \rangle\rangle \equiv \sum_{\text{triangles}} S_1(k_1, k_2, k_3) S_2(k_1, k_2, k_3). \quad (6.3)$$

Sometimes the configurations in this sum are weighted to approximate the sensitivity of a particular instrument, but `CppTransport` chooses to weight all configurations equally. With this choice the formal sum over triangles can be understood as an integral

$$\langle\langle B_1, B_2 \rangle\rangle \equiv \int dk_1 dk_2 dk_3 S_1(k_1, k_2, k_3) S_2(k_1, k_2, k_3). \quad (6.4)$$

For the reasons explained above this choice is not unique, and even when we have settled on a weighting for the integrand the definition must be completed by specifying UV and IR limits. The numerical value of a typical inner product $\langle\langle B_1, B_2 \rangle\rangle$ (and any conclusions that are drawn from it) will depend on the choices that are made. However, this arbitrariness is not really a cause for concern, because the purpose of the inner product is not mathematical but physical. Present-day experiments achieve only low signal-to-noise in measurements of any individual bispectrum configuration. Results with high signal-to-noise can be obtained only by supposing a relationship between the amplitude of different groups of configurations and averaging to obtain the cumulative contribution of the entire group. Our choice of inner product is useful if it happens that the averaging involved in Eq. (6.3) can be regarded as a proxy for the averaging over configurations performed by a realistic experiment.

6.5.1 The standard templates

CppTransport knows about a number of standard ‘templates’, or suppositions for the relationship between the amplitude of nearby bispectrum configurations. These are:

- **The local template.** This is defined by

$$B_{\zeta}^{\text{local}} = 2\left(P_{\zeta}(\mathbf{k}_1)P_{\zeta}(\mathbf{k}_2) + P_{\zeta}(\mathbf{k}_1)P_{\zeta}(\mathbf{k}_3) + P_{\zeta}(\mathbf{k}_2)P_{\zeta}(\mathbf{k}_3)\right). \quad (6.5)$$

- **The equilateral template.** This satisfies [58]

$$\begin{aligned} B_{\zeta}^{\text{equi}} = 6\left(& -P_{\zeta}(\mathbf{k}_1)P_{\zeta}(\mathbf{k}_2) - P_{\zeta}(\mathbf{k}_1)P_{\zeta}(\mathbf{k}_3) - P_{\zeta}(\mathbf{k}_2)P_{\zeta}(\mathbf{k}_3) \right. \\ & - 2[P_{\zeta}(\mathbf{k}_1)P_{\zeta}(\mathbf{k}_2)P_{\zeta}(\mathbf{k}_3)]^{2/3} \\ & \left. + [P_{\zeta}(\mathbf{k}_1)P_{\zeta}^2(\mathbf{k}_2)]^{1/3}P_{\zeta}(\mathbf{k}_3) + 5 \text{ cyclic permutations} \right) \end{aligned} \quad (6.6)$$

- **The orthogonal template.** This satisfies [59]

$$\begin{aligned} B_{\zeta}^{\text{ortho}} = 6\left(& -3P_{\zeta}(\mathbf{k}_1)P_{\zeta}(\mathbf{k}_2) - 3P_{\zeta}(\mathbf{k}_1)P_{\zeta}(\mathbf{k}_3) - 3P_{\zeta}(\mathbf{k}_2)P_{\zeta}(\mathbf{k}_3) \right. \\ & - 8[P_{\zeta}(\mathbf{k}_1)P_{\zeta}(\mathbf{k}_2)P_{\zeta}(\mathbf{k}_3)]^{2/3} \\ & \left. + 3[P_{\zeta}(\mathbf{k}_1)P_{\zeta}^2(\mathbf{k}_2)]^{1/3}P_{\zeta}(\mathbf{k}_3) + 5 \text{ cyclic permutations} \right) \end{aligned} \quad (6.7)$$

For any template B_{ζ}^i CppTransport defines an associated amplitude parameter f_{NL}^i ,

$$f_{\text{NL}}^i = \frac{5}{3} \frac{\langle\langle B, B_{\zeta}^i \rangle\rangle}{\langle\langle B_{\zeta}^i, B_{\zeta}^i \rangle\rangle} \quad (\text{no sum on } i) \quad (6.8)$$

When the inner products in (6.8) are a good estimate for the response of the quadratic estimator used for practical parameter estimation in a given experiment, the corresponding f_{NL}^i should be a good estimate for the amplitudes $f_{\text{NL}}^{\text{local}}$, $f_{\text{NL}}^{\text{equi}}$, $f_{\text{NL}}^{\text{ortho}}$ (and so on) measured by that experiment, assuming the true primordial bispectrum is B . On the other hand, if the inner product $\langle\langle \cdot, \cdot \rangle\rangle$ is not a good estimate for the response of a practical estimator then f_{NL}^i computed in this way may have little or nothing to do with the response of a real experiment. In particular, this can happen if B is too far from scale-invariant. The 3-dimensional inner product (6.3) will weight configurations near the upper limit k_{max} like k_{max}^3 , whereas a realistic CMB estimator working in ℓ space would weight such configurations like ℓ_{max}^2 . This difference in dimensionality can mean that $\langle\langle \cdot, \cdot \rangle\rangle$ overestimates the signal-to-noise contributed by the high- k configurations.

6.5.2 Building an inner-product task

To compute an inner product and associated f_{NL} -parameter for the double quadratic model we will need a new 3-point function task build from a linear grid. The output from this task should be attached to a ζ task, and the output from *that* should be attached to the inner-product task.

To specify the template the constructor for `fNL_task<>` requires a third argument. The possible values technically belong to CppTransport’s visualization toolkit rather than the underlying base platform, and therefore live in the `vis_toolkit` namespace rather than the `transport` namespace.

- `vis_toolkit::bispectrum_template::local` – local template
- `vis_toolkit::bispectrum_template::equilateral` – equilateral template
- `vis_toolkit::bispectrum_template::orthogonal` – orthogonal template

```

1 transport::basic_range<> ks_linearspaced(kt_lo, kt_hi, 50, transport::spacing::linear);
2
3 transport::threepf_cubic_task<> tk3_linear("dquad.threepf-linear", ics, ts, ks_linearspaced);
4 tk3_linear.set_adaptive_ics_efolds(4.0);
5 tk3_linear.set_description("Compute time history of the 3-point function on a linear grid");
6
7 transport::zeta_threepf_task<> ztk3_linear("dquad.threepf-linear-zeta", tk3_linear);
8 ztk3_linear.set_description("Convert the output from dquad.threepf-linear into zeta"
  ↪ " 2 and 3-point functions");
9
10 transport::fNL_task<> fNL_local("dquad.fNL-local", ztk3_linear,
  ↪ transport::bispectrum_template::local);
11 fNL_local.set_description("Compute inner product of double-quadratic bispectrum"
  ↪ " with local template");
12
13 repo.commit(fNL_local);

```

The resulting executable can be built in the usual way, and launched using `mpiexec`. We need only specify the final task `dquad.fNL-local`, because CppTransport will realise that content groups for `dquad.threepf-linear` and `dquad.threepf-linear-zeta` are required in order to generate suitable input.

With linear spacing in k we generate many more configurations, roughly 12,000. Although each configuration integrates fairly quickly, the total number means these tasks will take a few minutes to process:

```

1 $ mpiexec -n 4 dquad -v -r test-fNL --create --task dquad.fNL-local --gantt gantt-fNL.pdf
2 Task manager: processing task 'dquad.threepf-linear' (1 of 3)
3 Task manager: 2016-May-16 14:32:36
4 Items processed: 9073 In flight: 634 Remaining: 2344
5 Complete: 75.3% Mean CPU/item: 0.0985s Assignment: 60s
6 Estimated completion: 2016-May-16 14:34:26 (1m 50.7s from now)
7 Task manager: 2016-May-16 14:32:47
8 Items processed: 9707 In flight: 1196 Remaining: 1148
9 Complete: 80.5% Mean CPU/item: 0.0975s Assignment: 60s
10 Estimated completion: 2016-May-16 14:34:11 (1m 24.2s from now)
11 Task manager: 2016-May-16 14:33:50
12 Items processed: 10971 In flight: 868 Remaining: 212
13 Complete: 91% Mean CPU/item: 0.0969s Assignment: 60s
14 Estimated completion: 2016-May-16 14:34:30 (40.4s from now)
15 Task manager: 2016-May-16 14:34:08
16 All work items processed: 2016-May-16 14:34:08
17 Committed content group '20160516T132659' for task 'dquad.threepf-linear' at 2016-May-16 14:35:01
18 Task manager: processing task 'dquad.threepf-linear-zeta' (2 of 3)
19 Committed content group '20160516T133501' for task 'dquad.threepf-linear-zeta' at 2016-May-16
  ↪ 14:39:12
20 Task manager: processing task 'dquad.fNL-local' (3 of 3)
21 Committed content group '20160516T133912' for task 'dquad.fNL-local' at 2016-May-16 14:39:13
22 Task manager: processed 3 database tasks in wallclock time 12m 14.7s | time now 2016-May-16
  ↪ 14:39:13

```

On a slow filing system you may find that CppTransport's periodic progress updates show an adjustment of the target work assignment. For this task the final data container reaches ~ 3.5 Gb, and aggregation may take a few seconds per temporary database on an SSD, or

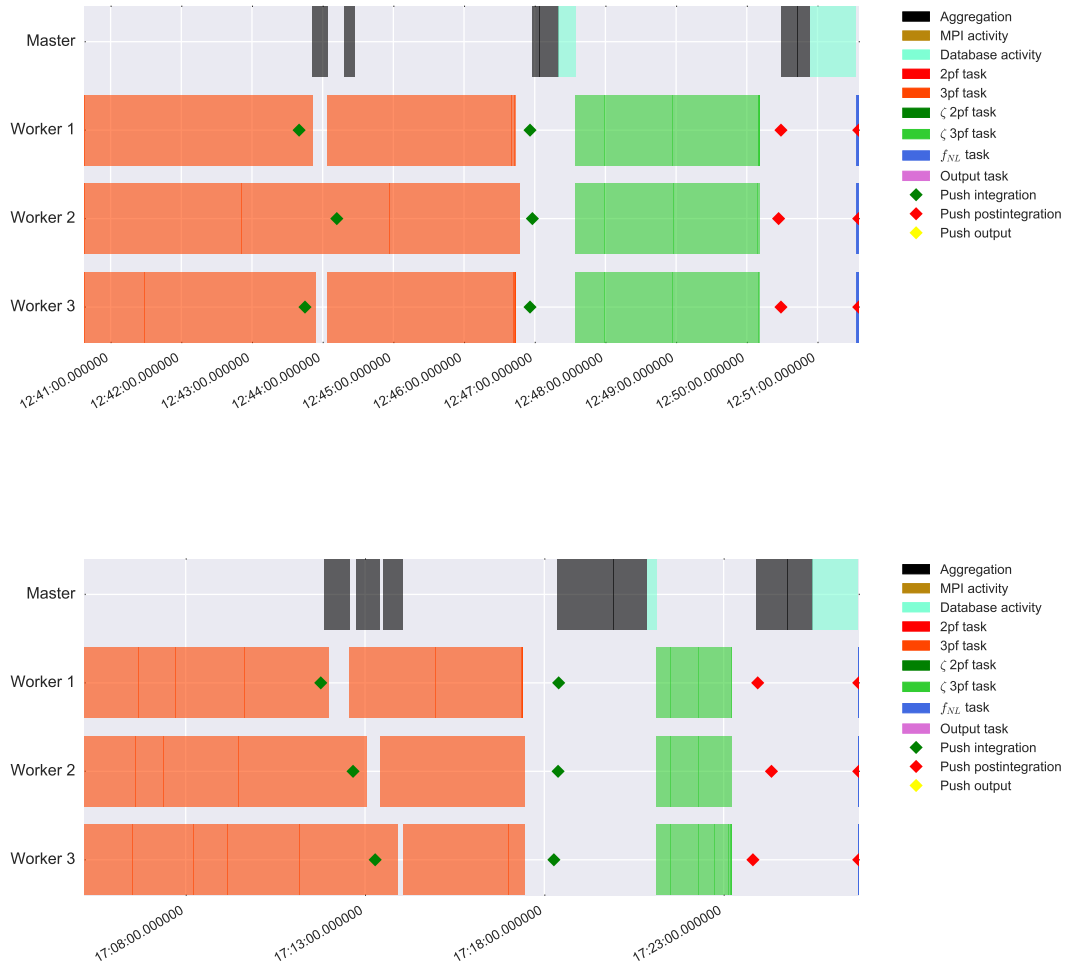


Figure 11. Process Gantt charts for the inner-product task `dquad.fNL-local`. Top chart: using a machine with solid-state storage. Bottom chart: using a machine with an external USB3 hard disk. Notice that aggregation is more time consuming using disks. Aggregation was performed using SQLite’s write-ahead logging mode.

more if writing to a conventional disk. As explained above, when aggregation times are non-negligible CppTransport schedules larger batches of work in an attempt to avoid wasteful stalls. That process Gantt chart for this job is shown in Fig. 11.

6.5.3 Example: Using the SQLite data container to produce a plot

In §7 we will see how to generate a derived product that plots the time history of f_{NL}^{local} in this model. As for other types of data-generating task, however, it is also possible to extract raw data from the SQLite database and use that directly.

Each inner-product task will write the following tables into its container:

1. `time_samples` – contains the list of time sample points. This table duplicates, and is inherited from, the one described in §4.8 (see p.64).

2. `fNL_local`

`fNL_equi`

`fNL_ortho` — contain the inner products needed to compute f_{NL}^i

Typically only one of these tables will be present, as appropriate. Each table contains the columns:

<code>tserial</code>	reference to serial number <code>time_samples.serial</code> identifying the time sample point for this row
<code>BB</code>	contains the inner product $\langle\langle B, B \rangle\rangle$, where B is the numerical bispectrum produced by the ζ task used as a source
<code>BT</code>	contains the inner product $\langle\langle B, T \rangle\rangle$, where B is as above and T is the appropriate template
<code>TT</code>	contains the inner product $\langle\langle T, T \rangle\rangle$

As an example, consider what would be required to compute f_{NL}^i from this database and plot it. The first step is to construct an SQL query that computes the required combination of the columns `BT` and `TT`. We also need a column representing the time sample point. A simple way to achieve this is

```
1 SELECT
2   tserial AS tserial,
3   (5 / 3) * BT / TT AS fNL
4 FROM fNL_local;
```

This is an example of the way in which short SQL queries can be used to perform simple data analysis without the need to write programs. For example, if we wished it would be possible to add a new column representing the (square of the) correlation ‘cosine’ between B and T ,

$$\cos^2(B, T) = \frac{\langle\langle B, T \rangle\rangle^2}{\langle\langle B, B \rangle\rangle \langle\langle T, T \rangle\rangle}. \quad (6.9)$$

To do this we would change the query:

```
1 SELECT
2   tserial AS tserial,
3   (5 / 3) * BT / TT AS fNL,
4   BT * BT / (BB * TT) AS cos_square
5 FROM fNL_local;
```

We would usually prefer to plot e-foldings N on the x -axis rather than the time serial number. This requires us to join the `fNL_local` and `time_samples` tables, by splicing together rows from each table to form a bigger table with more columns. This is accomplished by the SQL `INNER JOIN` clause:

```
1 SELECT
2   time_samples.time AS time,
3   (5 / 3) * fNL_local.BT / fNL_local.TT AS fNL,
4   fNL_local.BT * fNL_local.BT / (fNL_local.BB * fNL_local.TT) AS cos_square
5 FROM fNL_local
6   INNER JOIN time_samples ON fNL_local.tserial = time_samples.serial
7 ORDER BY time;
```

Most database managers will allow the results of this query to be saved in any suitable format. ‘Comma Separated Value’ or CSV is usually a good choice that has widespread support among third party tools. Once the data has been exported we can plot it as we

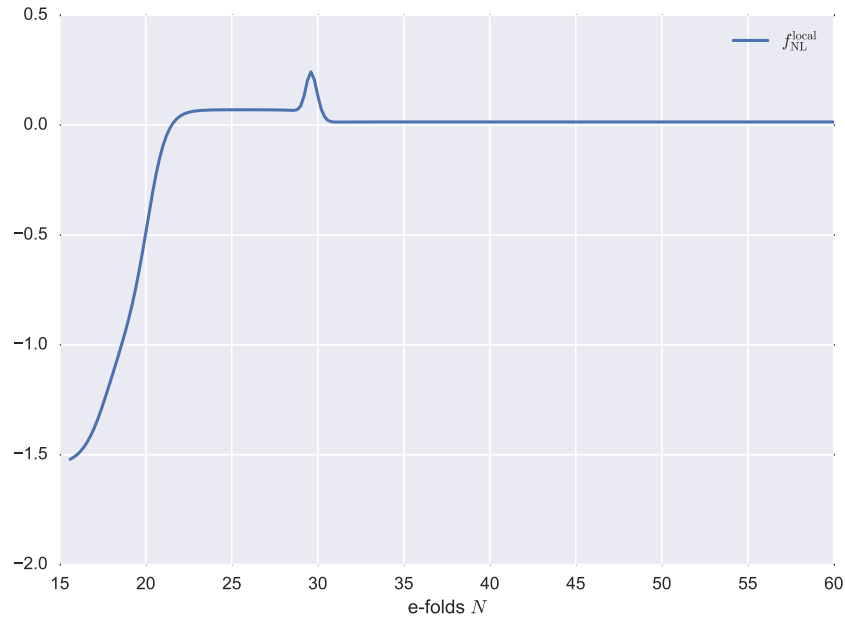


Figure 12. Evolution of the inner-product amplitude $f_{\text{NL}}^{\text{local}}$ in the double-quadratic inflation model.

wish, by using a suitable tool such as [Gnuplot](#). Alternatively, the following Python script will produce a simple plot from a CSV file.

```

1 import numpy as np
2 import matplotlib.pyplot as plt
3 import seaborn as sns
4 import csv
5
6 with open('fNL_local.csv') as f:
7     time = []
8     fNL_local = []
9
10    reader = csv.DictReader(f)
11    for row in reader:
12        time.append(float(row['time']))
13        fNL_local.append(float(row['fNL']))
14
15    time_data = np.array(time)
16    fNL_local_data = np.array(fNL_local)
17
18    plt.figure()
19    plt.plot(time_data, fNL_local_data, label='$f_{\mathrm{NL}}^{\mathrm{local}}$')
20
21    plt.xlabel(r'e-folds $N$')
22    plt.legend(frameon=False)
23    plt.savefig('fNL_local.pdf')

```

The resulting plot is shown in Fig. 12.

7 Generating derived products using output tasks

We are now in a position to consider the final step in performing an analysis with `CppTransport`—using its visualization toolkit to produce derived products. `CppTransport` can convert its raw n -point functions into a large number of derived quantities, some of which are observables. In many cases these quantities will be sufficient to undertake a simple model analysis, or comparison with summary observables such as the power spectrum amplitude or spectral index. For more advanced uses it may be preferable or necessary to export raw data from the database and process it using a dedicated pipeline.

The current implementation of the visualization toolkit can produce good quality two-dimensional line and scatter plots with minimal manual intervention. Outputs are built from a series of building blocks:

- **derived lines** are simple functions of time or configuration that can be extracted from the output of one or more tasks. Examples might be the values of raw correlation functions, the spectral index of the power spectrum, or the tensor-to-scalar ratio—all as functions of time or configuration. Many such quantities can be constructed using just one task but others require two, such as the tensor-to-scalar ratio. (The tensor amplitude is computed by a `twopf_task` or `threepf_task`, while the ζ amplitude is computed by the `zeta_*` versions of these.)
- **derived products** are groups of derived lines, presented either as a table or as a plot. A single derived product can include lines that draw data from many different integration or postintegration tasks. However, only groups of lines that share a common type of x -axis can be aggregated into a single derived product.
- **output tasks** are collections of derived products. When an output task is executed, `CppTransport` produces fresh copies of each derived product it contains. The standard rules described in §6.2 are used to select which content groups are used as data sources.

`CppTransport` supports two types of derived line: *time series*, which capture the evolution of some quantity as a function of e-foldings N , and *wavenumber series*, which capture the dependence on some aspect of the wavenumber configuration. This could be the scale k or k_t , but also shape parameters such as α or β , or the squeezing ratios k_i/k_t . It can automatically take derivatives of wavenumber series in order to measure spectral indices.

7.1 Selecting which data to plot using SQL query objects

To build a derived line requires selecting among the time and wavenumber samples stored by `CppTransport` during integration, or subsequently generated by a postintegration task. Because `CppTransport`'s internal data storage services are built on top of SQL databases, a natural and efficient means to perform this selection is to use SQL expressions as building blocks.

`CppTransport` provides three classes that encapsulate SQL expressions suitable for selecting a group of time or configuration sample points. `SQL_time_query` is used to select time samples, and `SQL_twopf_query` or `SQL_threepf_query` are used to select suitable configurations from the sample points for 2- or 3-point function wavenumber configurations. To use them, supply a suitable SQL expression based on the columns of the tables `time_samples`,

`twopf_samples` and `threepf_samples`, as appropriate. Each of these accepts a single argument, which is the SQL expression to use.

Selecting times.—For example, to build a trivial query that selects all configurations we require an expression that is always true, such as `1=1`. For example:

```
1 SQL_time_query all_times("1=1");
2 SQL_twopf_query all_twopfs("1=1");
3 SQL_threepf_query all_threepfs("1=1");
```

Alternatively, to select the latest time recorded in the database we could use

```
1 tserial IN (SELECT MAX(tserial) FROM time_samples)
```

The function `MAX` is provided by SQL. There is also a `MIN` function that can be used to select the earliest time available in the database, or we can combine these to get two sample points—both the earliest *and* latest times,

```
1 tserial IN (SELECT MAX(tserial) FROM time_samples UNION SELECT MIN(tserial) FROM time_samples)
```

To pick a specific time, it is possible to look up the corresponding serial number (using an HTML report as described in §4.4.2 for wavenumber configurations, but checking the time sample points instead) and specify it directly. Alternatively you can specify a range of times using a query such as `time > 10 AND time < 30`.

Selecting wavenumber configurations.—To select wavenumber configurations is equally easy. For 2-point function configurations we could select a range of wavenumbers using an expression such as

```
1 conventional > 10 AND conventional < 50
```

The available column names are those that apply to the corresponding SQL table, as described in §4.8. This means that we could also select configurations based on their horizon-exit time via the column `t_exit` or their massless point `t_massless`. So, for example, we could select all wavenumbers k that leave the horizon in some specified e-folding interval using

```
1 t_exit > 0.0 AND t_exit < 10.0
```

The same facilities are available for 3-point function configurations, for which it is possible to select on the columns `kt_conventional`, `kt_comoving`, `alpha`, `beta`, `t_exit_kt` or `t_massless`. If you wish to select on a squeezing ratio such as k_3/k_t then this has to be done by rewriting the expression in terms of α and β , eg. the SQL expression

```
1 (1-beta)/2 < 1E-3
```

will select all configurations with squeezing ratio $k_3/k_t < 10^{-3}$.

7.2 Example: plotting the evolution of the background fields

To see how these queries are used in practice, consider building a plot showing the time evolution of the background fields and their derivatives. To keep our function `write_tasks()` from becoming excessively long, we break it into two parts: one that builds the sample points and initial conditions, and another that builds tasks and derived products. Later, we will add further tasks and products; these can go in separate functions. Our prototypes are now

```

1 void write_tasks(transport::repository<>& repo, transport::dquad_mpi<>* model);
2
3 void write_zeta_products(transport::repository<>& repo, transport::initial_conditions<>& ics,
↪ transport::range<>& ts, transport::range<>& ks);

```

The function `write_tasks()` becomes

```

1 void write_tasks(transport::repository<>& repo, transport::dquad_mpi<>* model)
2 {
3     const double Mp = 1.0;
4     const double Mphi = 9E-5 * Mp;
5     const double Mchi = 1E-5 * Mp;
6
7     transport::parameters<> params(Mp, { Mphi, Mchi }, model);
8
9     const double phi_init = 10.0 * Mp;
10    const double chi_init = 12.9 * Mp;
11
12    const double N_init = 0.0;
13    const double N_pre = 12.0;
14    const double N_end = 60.0;
15
16    transport::initial_conditions<> ics("dquad", params, { phi_init, chi_init }, N_init, N_pre);
17
18    transport::basic_range<> ts(N_init, N_end, 300, transport::spacing::linear);
19
20    const double kt_lo = std::exp(3.0);
21    const double kt_hi = std::exp(8.0);
22
23    transport::basic_range<> ks_logspaced(kt_lo, kt_hi, 50, transport::spacing::log_bottom);
24    transport::basic_range<> ks_linearspaced(kt_lo, kt_hi, 50, transport::spacing::linear);
25
26    write_zeta_products(repo, ics, ts, ks_logspaced);
27 }

```

and the new function `write_zeta_products()` is

```

1 void write_zeta_products(transport::repository<>& repo, transport::initial_conditions<>& ics,
  ↪ transport::range<>& ts, transport::range<>& ks)
2 {
3     constexpr unsigned int num_fields = 2;
4
5     transport::threepf_cubic_task<> tk3("dquad.threepf", ics, ts, ks);
6     tk3.set_adaptive_ics_efolds(54.0);
7     tk3.set_description("Compute time history of the 3-point function on a cubic lattice"
  ↪ " from k ~ e^3 to k ~ e^9");
8
9     transport::zeta_threepf_task<> ztk3("dquad.threepf-zeta", tk3);
10    ztk3.set_description("Convert the output from dquad.threepf into zeta 2-"
  ↪ " and 3-point functions");
11
12    vis_toolkit::SQL_time_query all_times("1=1");
13
14    vis_toolkit::background_time_series<> bg_fields(tk3,
  ↪ vis_toolkit::index_selector<1>(num_fields).all(), all_times);
15
16    vis_toolkit::time_series_plot<> bg_plot("dquad.product.bg_plot", "background.pdf");
17    bg_plot.set_legend_position(vis_toolkit::legend_pos::bottom_left);
18    bg_plot += bg_fields;
19
20    transport::output_task<> out_tk("dquad.output.zeta");
21    out_tk += bg_plot;
22
23    repo.commit(out_tk);
24 }

```

The steps involved here are:

1. We set up a `threepf_cubic_task` and couple it to a `zeta_threepf_task` as described above. These tasks will collaborate to produce the raw n -point functions in the model.
2. We set up an `SQL_time_query` containing the trivial SQL query `1=1`. This will select all sample times stored in the database, so we will see the evolution of the background fields over the entire integration.

However, remember that with adaptive initial conditions, CppTransport will not begin storing samples until all n -point functions are available. This means that the first time stored in the database will be some time later than the initial time $N_{\text{init}} = 0$ specified in the initial conditions package `ics`.

3. We set up a time-series line for the background fields using the `vis_toolkit::background_time_series<>` class. Its constructor has signature

```

1 background_time_series(integration_task tk, index_selector<1> selector, SQL_time_query
  ↪ query)

```

The first argument identifies the integration task that will supply the data. The second argument is a new type of object, an `index_selector<>`. This determines which fields to plot. The final argument is an `SQL_time_query`. As explained above, this will determine which time sample points to include. Our choice `all_times` will use them all.

The constructor for the `index_selector` accepts a single argument, corresponding to the number of fields in the model. It takes a template argument between angle brackets, here `<1>`, to indicate the number of indices being selected from. For example: the

background fields have one index, the two-point function Σ^{ab} has two indices, and the three-point function α^{abc} has three indices.

By default all components are selected, but to be explicit we have used the `all()` method to indicate that they should all be included. This will give us a plot showing the field expectation values $\phi(N)$, $\chi(N)$ and also their derivatives $p_\phi \equiv d\phi/dN$ and $p_\chi = d\chi/dN$.

4. Once the derived line has been created we build a plot to contain it. This is the object `time_series_plot<>`. Its constructor takes two arguments: a *derived product name* (which should be unique) and a filename. The format of the output file is inferred by Matplotlib from the extension of the filename. Any format that can be written by Matplotlib may be used, and typically PDF (`.pdf`) or SVG (`.svg`) are good for plots. As an alternative it is possible to specify a filename with extension `.py`. This causes CppTransport to write a Python script that will produce the plot, but it does not execute it—the script *is* the derived product. This gives an opportunity to apply custom formatting or to apply adjustments that CppTransport cannot make automatically.
5. By default, the plot includes a legend that is placed in the upper right-hand corner. In this case it will overlay the lines, so we elect to move it to the bottom left-hand corner using the `set_legend_position()` method.
6. The data line `bg_fields` is added to the plot by writing `bg_plot += bg_fields`. If we had more than one line to add we could include them all in a summation on the right-hand side.
7. Finally, we build an output task called `dquad.output.zeta`. We add the plot to the task by writing `out_tk += bg_plot`. The output task is committed to the database. Notice that there is no need to commit the derived products on which the task depends, or the tasks on which those derived products depend, because CppTransport will automatically commit these dependencies if they are required.

To test, build the executable and launch the task `dquad.output.zeta` using

```
1 $ mpiexec -n 4 dquad -v -r test-output --create --task dquad.output.zeta
```

As usual, CppTransport will schedule execution of any tasks needed to produce content groups that feed later tasks in the chain:

```
Task manager: processing task 'dquad.threepf' (1 of 2)
Committed content group '20160516T135141' for task 'dquad.threepf' at 2016-May-16 15:00:18
Task manager: processing task 'dquad.output.zeta' (2 of 2)
Committed content group '20160516T140133' for task 'dquad.output.zeta' at 2016-May-16 15:01:43
Task manager: processed 2 database tasks in wallclock time 10m 1.8s | time now 2016-May-16 15:01:43
```

Fig. 13 shows the generated plot, using the `seaborn` plot style. We will discuss its features below and explain how it can be customized.

CppTransport employs a similar directory structure to that used for integration and postintegration tasks. Generated content is placed in the output folder of the repository, under a subfolder with name corresponding to the output task. Inside this folder, each content group is placed in a directory with name given by the content group name. Each

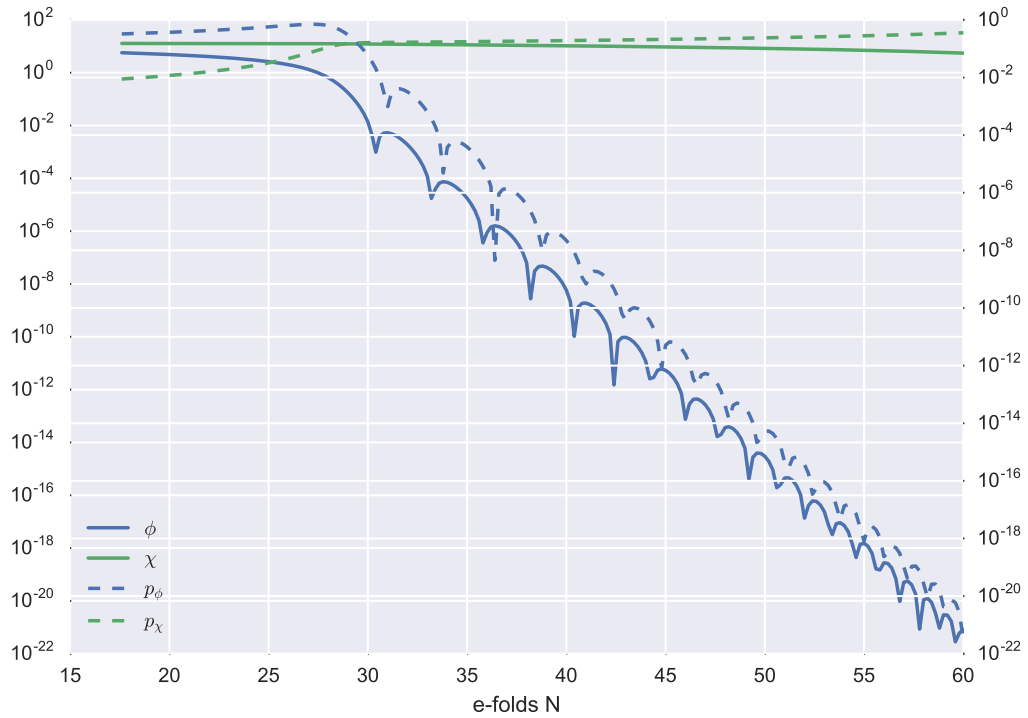


Figure 13. Time evolution of background fields ϕ , χ and their derivatives p_ϕ , p_χ generated by the produce `dquad.product.bg_plot`.

derived product is generated inside this directory, with the filename specified when the derived product was set up. There is also the usual logs folder that contains detailed logging from the master and worker processes while the task was in progress.

Reporting on output content groups.—Asking CppTransport to report on `dquad.output.zeta` shows the derived products that are generated as part of the task, and lists each associated content group:

```

1  $ ./dquad -r test-output/ --info dquad.output.zeta
2  dquad.output.zeta -- output task
3  Created: 2016-May-16 13:51:40      Last update: 2016-May-16 14:01:43
4  Runtime version: 2016.1
5
6  Derived product                    Type    Matches tags  Filename
7  dquad.product.bg-plot              2d plot  --            background.pdf
8
9  Content group                      Created      Last update
10  20160516T140133    2016-May-16 14:01:33  2016-May-16 14:01:43

```

If we instead report on the content group generated by this task, CppTransport will summarize the content groups that were used to feed data into its derived products:

```

1 $ ./dquad -r test-output/ --info 20160516T140133
2 20160516T140133 -- derived content
3 Created: 2016-May-16 14:01:33      Last update: 2016-May-16 14:01:43
4 Runtime version: 2016.1           Task: dquad.output.zeta
5 Locked: No                         Tags: --
6
7 Summary of content groups used
8 Content group  Task                Type                Last update
9 20160516T135141 dquad.threepf      integration         2016-May-16 14:00:18

```

The table aggregates all dependencies, but sometimes it is more useful to see individually how each derived product depends on other content groups. `CppTransport` can provide this information as a *provenance report*, obtained by using the command-line option `--provenance` rather than `--info`.

The same information is embedded in an HTML report, and often these are the easiest way to navigate the network of dependencies. Content groups generated by output tasks are listed under the ‘Output content’ tab, and where possible the report includes any generated plots. This is often a good way to view the products generated by an output task, especially if there are more than a few. See Fig. 14. The report for each derived product includes a table of dependencies similar to that provided by the `--provenance` option. Also, if `Graphviz` is installed, it will produce a dependency diagram showing the interrelation of initial conditions packages, tasks and content groups that yielded the data for this product. An example for the background fields plot is shown in Fig. 15.

7.3 Derived products: plots and tables

The current implementation of the visualization toolkit supports four principal types of derived product:

- The products `time_series_plot<>` and `wavenumber_series_plot<>` are two-dimensional graphs suitable for plotting time-series and wavenumber-series data, respectively.
- The products `time_series_table<>` and `wavenumber_series_table<>` are suitable for tabulating time- and wavenumber-series data.

The constructors for these derived products have a standard signature consisting of two arguments: a unique name, and an output filename. We have already seen this in action for the `time_series_plot<>` used to plot background field data above.

7.3.1 Standard options

Each derived product can be customized by applying options. The `set_*` methods can be chained together for more economical expression.

- `bool get_log_x()`
`set_log_x(bool f)`
Determine whether logarithmic *x*-axis values are used, if this makes sense for the product. Off by default.
- `bool get_log_y()`
`set_log_y(bool f)`
Determine whether logarithmic *y*-axis values are used, if this makes sense for the product. Enabled by default for plots.

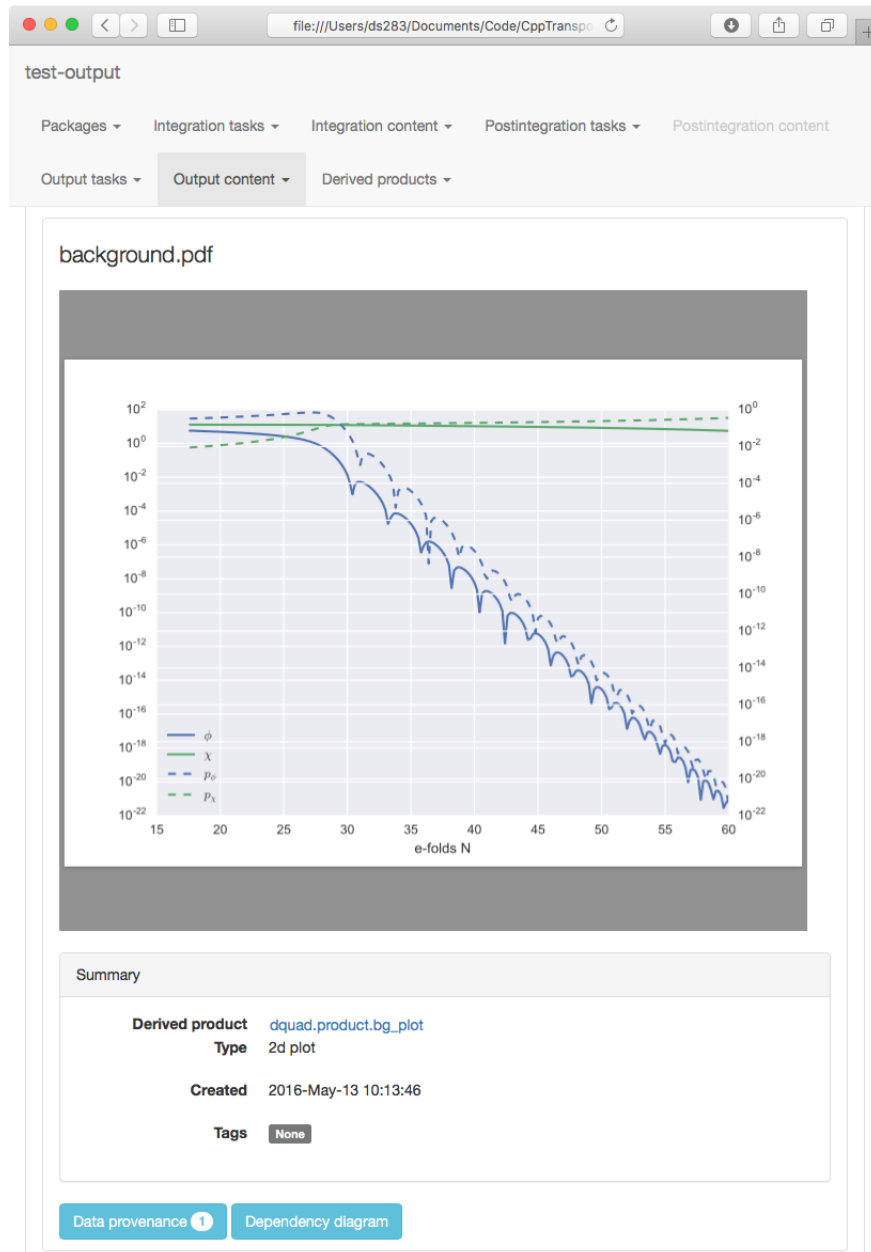


Figure 14. The HTML report for content groups generated by output tasks will include the output where possible. Click the ‘Data provenance’ button to display a hyperlinked list of content groups showing the data sources for each product. The ‘Dependency diagram’ shows how the data sources depend on each other, on particular integration and postintegration tasks, and ultimately on a set of initial conditions packages.

- `bool get_abs_y()`
`set_abs_y(bool f)`

Determine whether absolute y -values are used. Enabled by default for plots.

If a logarithmic y -axis is in use, CppTransport will detect whether absolute values are

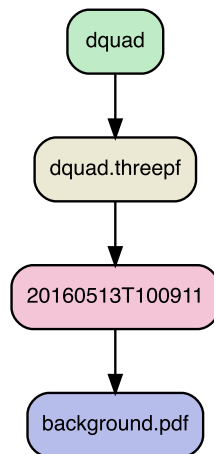


Figure 15. Dependency diagram for the background field plot `dquad.products.bg_plot`. In this case the chain of dependencies is very straightforward, but more complex cases are possible. Initial conditions packages are coloured green, tasks are coloured yellow, content groups are red and derived products are blue.

needed for lines that have negative values.

- `bool get_use_LaTeX()`
`set_use_LaTeX()`

Determine whether \LaTeX -format labels are used in preference to plain text. Notice that this has nothing to do with whether \LaTeX is involved in typesetting. Enabled by default for plots.

7.3.2 Plot-specific options

In addition, there are a number of options that are specific to plots, ie. the objects `time_series_plot<>` and `wavenumber_series_plot<>`. As usual, the `set_*` methods can be chained.

Axis handling.—The following options influence axes:

- `bool get_reverse_x()`
`set_reverse_x(bool)`

Determine whether x -axis is reversed. Off by default.

- `bool get_reverse_y()`
`set_reverse_y(bool)`

Determine whether y -axis is reversed. Off by default.

Labelling.—The following options determine labelling:

- `bool get_x_label()`
`set_x_label(bool)`

Determine whether a label is added to the x -axis. Enabled by default.

- `std::string get_x_label_text()`
`set_x_label_text(std::string)`
`clear_x_label_text()`

Set or clear text for x -axis label, if it is in use. Does not imply labelling is enabled.

If labelling is enabled but no text is explicitly supplied, `CppTransport` will use a default label. In this case, `get_x_label_text()` will return an empty string.

- `bool get_y_label()`
`set_y_label(bool)`

Determine whether a label is added to the y -axis. Off by default.

On the example of Fig. 13 we could switch on labelling on the y -axis by adding

```
1 bg_fields.set_y_label(true);
```

before adding the `bg_fields` lines to `bg_plot`. It is not necessary to specify a label; `CppTransport` will apply default labels based on quantities represented by each axis. If we wish, however, it is possible to specify a label using the `set_y_label_text` method described below. This sets the label for the first axis only.

- `std::string get_y_label_text()`
`set_y_label_text(std::string)`
`clear_y_label_text()`

Set or clear text for y -axis label, if it is in use. Does not imply labelling is enabled.

If labelling is enabled but no text is explicitly supplied, `CppTransport` will use a default label. In this case, `get_y_label_text()` will return an empty string.

- `bool get_title()`
`set_title(bool)`

Determine whether a title is added to the plot. Off by default.

- `std::string get_title_text()`
`set_title_text(std::string)`
`clear_title_text()`

Set or clear text for plot title, if it is in use. Does not imply titling is enabled.

If no title text has been supplied, `get_title_text()` will return an empty string.

- `bool get_legend()`
`set_legend(bool)`

Determine whether a legend is included on the plot. Enabled by default.

- `vis_toolkit::legend_pos get_legend_position()`
`set_legend_position(vis_toolkit::legend_pos)`

Determine position of legend, if one is enabled. By default the legend is position in the top right corner of the plot

The allowed values are:

<code>vis_toolkit::legend_pos::top_left</code>	legend in top left corner
<code>vis_toolkit::legend_pos::top_right</code>	legend in top right corner
<code>vis_toolkit::legend_pos::bottom_left</code>	legend in bottom left corner
<code>vis_toolkit::legend_pos::bottom_right</code>	legend in bottom right corner
<code>vis_toolkit::legend_pos::right</code>	legend position to right of plot
<code>vis_toolkit::legend_pos::centre_right</code>	legend in right side of plot, vertically centred
<code>vis_toolkit::legend_pos::centre_left</code>	legend in left side of plot, vertically centred
<code>vis_toolkit::legend_pos::upper_centre</code>	legend in top of plot, horizontally centred
<code>vis_toolkit::legend_pos::lower_centre</code>	legend in bottom of plot, horizontally centred
<code>vis_toolkit::legend_pos::centre</code>	legend in centre of plot

- `bool get_typeset_with_LaTeX()`
`set_typeset_with_LaTeX(bool)`

Determine whether `Matplotlib` is asked to offload typesetting responsibilities to `LATEX`. This produces higher quality results but is slower, and requires a `LATEX` toolchain to be installed on the current user's `PATH`. `LATEX` is needed for some typesetting choices because `Matplotlib`'s built-in typesetting engine does not support the full range of `LATEX` commands.

Disabled by default. Notice that this setting is independent of whether `LATEX`-format labels have been enabled using `set_use_LaTeX()`.

- `bool get_dash_second_axis()`
`set_dash_second_axis(bool)`

Determine whether lines associated with a second vertical axis are distinguished by being dashed. `CppTransport` understands that different derived products have different units and scales, and where necessary it will add a second axis to handle lines with two different intrinsic scales. An example is the plot of background fields already produced in Fig. 13. Here, although the axes are not labelled in the default configuration, the left-hand vertical axis refers to the value of the fields ϕ , χ and the right-hand axis refers to the value of their derivatives.

To disable dashing on our example plot Fig. 13 we should add

```
1 bg_fields.set_dash_second_axis(false);
```

before adding `bg_fields` to the plot `bg_plot`.

Enabled by default.

7.3.3 Table-specific options

For the table objects `time_series_table<>` and `wavenumber_series_table<>` there is an option to select the table format:

- `vis_toolkit::table_format get_format()`
`set_format(vis_toolkit::table_format f)`

Determine the format of the table. The allowed options are:

<code>vis_toolkit::table_format::justified</code>	aligned in columns, padded with spaces
<code>vis_toolkit::table_format::csv</code>	comma-separated value
<code>vis_toolkit::table_format::tsv</code>	tab-separated value

The default format is determined from the filename extension. If this is `.csv` or `.tsv` then the format is set to CSV or TSV respectively. The other allowed formats are `.txt`, `.data` and `.dat`. These use justified output.

7.4 Available derived lines

In this section we document the different derived lines provided by the visualization toolkit. Each line is represented by a suitable object whose constructor typically requires:

- one or more **task objects** that specify the data sources for the line
- for lines representing tensor objects such as the two-point function Σ^{ab} or the three-point function α^{abc} , an **index selector** that specifies which components should be plotted
- for both time-series and wavenumber-series objects, two **SQL query expressions**—one for time configurations, and another for wavenumber configurations.
 - for *time series*, the time query determines the range of points sampled on the x -axis. If the wavenumber-configuration query generates multiple points then these are used to produce different lines on the plot.
 - for *wavenumber series* the situation is reversed. The wavenumber configuration query determines the points sampled on the x -axis, and if the time query generates multiple points then these are plotted as multiple lines.

7.4.1 Standard options

In addition, each line has a number of standard options. These settings are available for all derived lines, although not every line will make use of each option.

- `vis_toolkit::dot_type get_dot_meaning()`
`set_dot_meaning(vis_toolkit::dot_type)`

Determines whether the phase space is taken to be built from the fields and their derivatives with respect to N , or the fields and their canonical momenta.

The allowed values for `vis_toolkit::dot_type` are:

<code>vis_toolkit::dot_type::derivatives</code>	use derivatives
<code>vis_toolkit::dot_type::momenta</code>	use momenta

This setting affects only derived products containing field space correlation functions.

- `vis_toolkit::klabel_type get_klabel_meaning()`
`set_klabel_meaning(vis_toolkit::klabel_type)`

Determines whether conventional or comoving momenta are used.

The allowed values for `vis_toolkit::klabel_type` are:

<code>vis_toolkit::klabel_type::conventional</code>	use conventional normalization
<code>vis_toolkit::klabel_type::comoving</code>	use comoving normalization

The comoving normalization is the one set by the value of a_* ; see p.69.

- `vis_toolkit::axis_value get_current_x_axis_value()`
`set_current_x_axis_value(vis_toolkit::axis_value)`

Determines how the x -axis is constructed.

CppTransport can use several different quantities for the x -axis scale:

<code>vis_toolkit::axis_value::efolds</code>	use e-folds N
<code>vis_toolkit::axis_value::k</code>	use wavenumber k (or k_t for 3-point function data)
<code>vis_toolkit::axis_value::efolds_exit</code>	use e-folds between N_* and horizon exit of wavenumber k (or $k_t/3$ for 3-point function data)
<code>vis_toolkit::axis_value::alpha</code>	use the shape parameter α
<code>vis_toolkit::axis_value::beta</code>	use the shape parameter β
<code>vis_toolkit::axis_value::squeeze_k1</code>	
<code>vis_toolkit::axis_value::squeeze_k2</code>	
<code>vis_toolkit::axis_value::squeeze_k3</code>	use the squeezing ratio k_i/k_t

Not all derived lines support all x -axis types. Time series lines support only `efolds`, and wavenumber series associated with configurations of the 2-point function support only `k` and `efolds_exit`. Wavenumber series associated with configurations of the 3-point function support all types except `efolds`. CppTransport will raise an exception if you attempt to select an unsupported x -axis value.

Derived products can contain only lines with the same x -axis type. If you attempt to add lines with different types to the same product then CppTransport will raise an exception.

- `clear_label_text()`
`set_label_text(std::string latex, std::string non_latex)`

Set or clear a customized label for this line.

Two labels are required: one in L^AT_EX format and one in plain text format. The L^AT_EX-format label is used if L^AT_EX labels have been enabled by `set_use_LaTeX()` (see §7.3.1). Otherwise, the plain text label is used.

Labels are used as column headings (if the derived product is a table) or displayed on the legend (if the derived product is a plot). If no label is set then CppTransport will use a suitable default.

- `bool get_label_tags()`
`set_label_tags(bool)`

Determine whether identifying ‘tags’ are added to each label. For time series, the tag identifies the wavenumber configuration corresponding to each line (if relevant). For wavenumber series it identifies the time sample point.

Tags are useful where a single derived line generates multiple physical lines and you wish to distinguish them.

7.4.2 Options for 2-point correlation functions

The lines representing 2-point correlation functions are:

- `twopf_time_series`
- `twopf_wavenumber_series`
- `tensor_time_series`
- `tensor_wavenumber_series`
- `zeta_twopf_time_series`
- `zeta_twopf_wavenumber_series`

These lines have additional options:

- `set_dimensionless(bool)`
Determine whether the dimensionful or dimensionless correlation function is plotted. The dimensionless correlation function \mathcal{P} is defined in terms of the dimensionful correlation function Σ via

$$\mathcal{P} = \frac{k^3}{2\pi^2} \Sigma. \quad (7.1)$$

Enabled by default.

The field-space two-point function lines `twopf_time_series` and `twopf_wavenumber_series` have an additional option that allows them to be switched between real and imaginary values, where available.

- `vis_toolkit::twopf_type get_type()`
`set_type(vis_toolkit::twopf_type)`

Determine whether real or imaginary values are used.

The allowed values of `vis_toolkit::twopf_type` are:

<code>vis_toolkit::twopf_type::real</code>	use real values
<code>vis_toolkit::twopf_type::imaginary</code>	use imaginary values

Real values are used by default. Notice that only datasets generated by three-point function tasks include imaginary values for the 2-point function.

7.4.3 Options for 3-point correlation functions

The lines representing 3-point correlation functions are:

- `threepf_time_series`
- `threepf_wavenumber_series`
- `zeta_threepf_time_series`

- `zeta_threepf_wavenumber_series`

These lines have additional options:

- `set_dimensionless(bool)`

Determine whether the dimensionful or dimensionless correlation function is plotted. The dimensionless correlation function S^{abc} is sometimes called the shape function. It is defined in terms of the dimensionful 3-point function α by

$$S = (k_1 k_2 k_3)^2 \alpha. \quad (7.2)$$

Enabled by default.

- `bool get_use_kt_label()`
`set_use_kt_label(bool)`

If tags are being attached to labels (see p.99), determine whether the k_t value is used as part of the label. Enabled by default.

- `bool get_use_alpha_label()`
`set_use_alpha_label(bool)`

If tags are being attached to labels (see p.99), determine whether the α shape parameter is used as part of the label. Disabled by default.

- `bool get_use_beta_label()`
`set_use_beta_label(bool)`

If tags are being attached to labels (see p.99), determine whether the β shape parameter is used as part of the label. Disabled by default.

If your configurations vary only with scale k_t then the default tag will be correct. However, if you are varying more than one parameter, or keeping k_t constant while varying α or β , you should consider changing which quantities are used to generate the tag.

In addition, the ‘reduced bispectrum’ (6.2) is defined by a ratio of 2- and 3-point correlation functions. It is represented by the lines

- `zeta_reduced_bispectrum_time_series`
- `zeta_reduced_bispectrum_wavenumber_series`

They have the same options given above except for `set_dimensionless()`.

7.4.4 Time series

This section lists the available time series lines and the signature of their constructors. As a shorthand, the namespace `vis_toolkit` is omitted for the names of the lines themselves, and for types appearing in their constructors such as `vis_toolkit::SQL_time_query` and `vis_toolkit::index_selector<>`. We also use the following abbreviations for task types:

<code>integration_task</code>	any integration task
<code>threepf_task</code>	any 3-point function integration task
<code>zeta_task</code>	any ζ postintegration task
<code>zeta_threepf_task</code>	a ζ 3-point function task
<code>fNL_task</code>	any f_{NL} postintegration task

Each time series requires an `vis_toolkit::SQL_time_query` to select the time sample points. Each sample is taken at fixed wavenumber configuration, selected by a `vis_toolkit::SQL_twopf_query` or `vis_toolkit::SQL_threepf_query` that must also be supplied. Where this query picks out multiple configurations, they are included as separate columns in a table or lines in a plot.

- `background_time_series<>`

Time evolution of the background fields and their derivatives.

```
1 background_time_series(
2   integration_task,
3   index_selector<1>,
4   SQL_time_query
5 )
```

- `twopf_time_series<>`

Time evolution of the field-space two-point correlation function Σ^{ab} (or its dimensionless counterpart).

```
1 twopf_time_series(
2   integration_task,
3   index_selector<2>,
4   SQL_time_query,
5   SQL_twopf_query
6 )
```

- `threepf_time_series<>`

Time evolution of the field-space three-point correlation function α^{abc} (or its dimensionless counterpart).

```
1 threepf_time_series(
2   threepf_task,
3   index_selector<3>,
4   SQL_time_query,
5   SQL_twopf_query
6 )
```

- `tensor_time_series<>`

Time evolution of the tensor two-point correlation function $\Sigma_{ss'}$ (or its dimensionless counterpart).

```
1 tensor_time_series(
2   integration_task,
3   index_selector<2>,
4   SQL_time_query,
5   SQL_twopf_query
6 )
```

- `r_time_series<>`

Time evolution of the tensor-to-scalar ratio r .

```

1 r_time_series(
2     zeta_task,
3     SQL_time_query,
4     SQL_twopf_query
5 )

```

- `zeta_twopf_time_series<>`

Time evolution of the ζ two-point correlation function Σ_ζ (or its dimensionless counterpart).

```

1 zeta_twopf_time_series(
2     zeta_task,
3     SQL_time_query,
4     SQL_twopf_query
5 )

```

- `zeta_threepf_time_series<>`

Time evolution of the ζ three-point correlation function α_ζ (or its dimensionless counterpart).

```

1 zeta_threepf_time_series(
2     zeta_threepf_task,
3     SQL_time_query,
4     SQL_twopf_query
5 )

```

- `zeta_reduced_bispectrum_time_series<>`

Time evolution of the ζ reduced bispectrum, defined by Eq. (6.2).

```

1 zeta_reduced_bispectrum_time_series(
2     zeta_threepf_task,
3     SQL_time_query,
4     SQL_twopf_query
5 )

```

- `fNL_time_series<>`

Time evolution of an inner product amplitude f_{NL}^i ; see Eq. (6.8).

```

1 fNL_time_series(
2     fNL_task,
3     SQL_time_query
4 )

```

- `background_line<>`

Time evolution of a background quantity. Currently-implemented options are H , ϵ and aH .

```

1 background_line(
2     integration_task,
3     SQL_time_query,
4     background_quantity
5 )

```

The allowed values of `vis_toolkit::background_quantity` are:

<code>vis_toolkit::background_quantity::epsilon</code>	compute $\epsilon = -\dot{H}/H^2$
<code>vis_toolkit::background_quantity::Hubble</code>	compute Hubble parameter H
<code>vis_toolkit::background_quantity::aH</code>	compute comoving Hubble scale aH

- `u2_line<>`

Time evolution of components of the tensor u_{ab} .

```
1 u2_line(  
2     integration_task,  
3     index_selector<2>,  
4     SQL_time_query,  
5     SQL_twopf_query  
6 )
```

- `u3_line<>`

Time evolution of components of the tensor u_{abc} .

```
1 u3_line(  
2     threepf_task,  
3     index_selector<2>,  
4     SQL_time_query,  
5     SQL_threepf_query  
6 )
```

Notice that because u_{abc} is a function of a bispectrum configuration it can be computed only for 3-point function integrations.

- `largest_u2_line<>`

Time evolution of the largest component of the momentum-field block of u_{ab} , which is numerically equivalent to the field-space mass matrix in Hubble units $M_{\alpha\beta}/H^2$. The other components of u_{ab} have fixed magnitudes or depend only on ϵ , and so are excluded.

```
1 largest_u2_line(  
2     integration_task,  
3     index_selector<2>,  
4     SQL_time_query,  
5     SQL_twopf_query  
6 )
```

- `largest_u3_line<>`

Time evolution of the largest component of u_{abc} . Unlike u_{ab} , *all* components are included.

```
1 largest_u3_line(  
2     threepf_task,  
3     index_selector<3>,  
4     SQL_time_query,  
5     SQL_threepf_query  
6 )
```

7.4.5 Wavenumber series

For each quantity that is wavenumber-configuration dependent there is a corresponding wavenumber series. We describe these using the same conventions used for time series in §7.4.4.

Like the corresponding time series, each wavenumber series requires a `vis_toolkit::SQL_time_query` and one or other of `vis_toolkit::SQL_twopf_query` or `vis_toolkit::SQL_threepf_query`. For wavenumber series, the twopf- or threepf-query is used to select the sample points that will appear on the x -axis and the time query selects the particular time at which we wish to sample. If multiple times are included, they generate separate columns in a table or lines on a plot.

Spectral indices.—All wavenumber series have an extra option to compute the spectral index, using the current x -axis type; the definition is

$$n = \frac{d \ln y}{d \ln x}. \quad (7.3)$$

If y can be approximated as a slowly varying power law, then n can be regarded as an estimate for the power-law index $y \sim x^n$. For example, if x is a wavenumber and y is a power spectrum, then n computed in this way is the usual spectral index. Alternatively, if y is a reduced bispectrum and x is a squeezing ratio k_i/k_t then n gives the local approximate power law $f_{\text{NL}}(k_1, k_2, k_3) \sim (k_i/k_t)^n$.

The calculation of spectral indices is enabled using `set_spectral_index(bool)`.

Warning

When computing spectral indices associated with variation of the bispectrum configuration, as above, it is important to be careful about which quantities vary and which are held fixed.

For example, to measure the spectral index associated with variations of the squeezing k_i/k_t at fixed scale, we should keep k_t fixed. The SQL query expression that selects those configurations to include should enforce this constraint.

Likewise, to measure the spectral index associated with variations of scale k_t we should usually keep the squeezing parameters k_i/k_t fixed.

Warning

In the current version of `CppTransport`, spectral indices generated using this option should be treated with caution. The calculation is performed by fitting a spline to $y(x)$ and differentiating this spline.

In general this gives acceptable results, but there are some pitfalls. First, the spline and its derivative can lose accuracy near the edges of the fitted region. This tends to introduce some spurious jitter into the spectral index. Second, with a large number of sample points the spline tends to be overfit. `CppTransport` tries to compensate for this by using a p -spline (a ‘penalized’ spline that tries to smoothly interpolate between sample points, rather than strictly passing through each point), but it is not always successful.

For these reasons it is wise to check the spectral index calculation using other methods before relying on the result.

- `twopf_wavenumber_series<>`

k -dependence of the field-space two-point correlation function Σ^{ab} (or its dimensionless counterpart).

```
1 twopf_wavenumber_series(  
2     integration_task,  
3     index_selector<2>,  
4     SQL_time_query,  
5     SQL_twopf_query  
6 )
```

- `threepf_wavenumber_series<>`

Configuration-dependence of the field-space three-point correlation function α^{abc} (or its dimensionless counterpart).

```
1 threepf_wavenumber_series(  
2     threepf_task,  
3     index_selector<3>,  
4     SQL_time_query,  
5     SQL_twopf_query  
6 )
```

- `tensor_wavenumber_series<>`

k -dependence of the tensor two-point correlation function $\Sigma_{ss'}$ (or its dimensionless counterpart).

```
1 tensor_wavenumber_series(  
2     integration_task,  
3     index_selector<2>,  
4     SQL_time_query,  
5     SQL_twopf_query  
6 )
```

- `r_wavenumber_series<>`

k -dependence of the tensor-to-scalar ratio r .

```
1 r_time_series(  
2     zeta_task,  
3     SQL_time_query,  
4     SQL_twopf_query  
5 )
```

- `zeta_twopf_wavenumber_series<>`

k -dependence of the ζ two-point correlation function Σ_ζ (or its dimensionless counterpart).

```

1  zeta_twopf_wavenumber_series(
2      zeta_task,
3      SQL_time_query,
4      SQL_twopf_query
5  )

```

- `zeta_threepf_wavenumber_series<>`

Configuration-dependence of the ζ three-point correlation function α_ζ (or its dimensionless counterpart).

```

1  zeta_threepf_wavenumber_series(
2      zeta_threepf_task,
3      SQL_time_query,
4      SQL_twopf_query
5  )

```

- `zeta_reduced_bispectrum_wavenumber_series<>`

Configuration-dependence of the ζ reduced bispectrum, defined by Eq. (6.2).

```

1  zeta_reduced_bispectrum_time_series(
2      zeta_threepf_task,
3      SQL_time_query,
4      SQL_twopf_query
5  )

```

7.4.6 Integration cost analysis

Finally, a special set of derived lines exist that do not represent data or observables, but rather provide metadata about the performance of the integration. These can be used to provide more targeted versions of the scatter plots generated by HTML reports and discussed in §4.7.1. (See Fig. 9.) These automatically-generated plots include all configurations, whereas the derived lines offer more control through the use of SQL query expressions to restrict the configuration that are included.

- `cost_wavenumber<>`

Supply the per-configuration integration cost, where this information is available.

```

1  cost_wavenumber(
2      twopf_task,
3      SQL_twopf_query,
4      cost_metric
5  )
6
7  cost_wavenumber(
8      threepf_task,
9      SQL_threepf_task,
10     cost_metric
11 )

```

The allowed values of `vis_toolkit::cost_metric` are

<code>vis_toolkit::cost_metric::time</code>	measure integration time
<code>vis_toolkit::cost_metric::steps</code>	measure number of steps taken by stepper

7.5 Enabling or disabling indices using an `index_selector<>`

In §§7.2–7.4 it was explained that for derived lines generated by objects with multiple indices, a `index_selector<>` object must be supplied to select which indices should be included.

Constructing a selector requires specifying a template argument that fixes the number of indices. The constructor accepts a single argument giving the number of fields. For example, to build a selector for a 2-index object such as the field-space correlation function Σ^{ab} , we could use

```
1 vis_toolkit::index_selector<2> sel(num_fields);
```

where `num_fields` should be suitably defined. (It could be extracted from the `get_N_fields()` method of a `transport::model` object, which returns the number of fields used in the model.)

Index selectors enable all components by default. Once constructed, a selector provides methods `all()` and `none()` that explicitly enable or disable all components. It is also possible to enable or disable individual components by supplying a tuple of numbers representing the component in question. As in the mapping used for index assignment in SQLite containers, fields are assigned increasing integers beginning at 0 and with ordering inherited from the model description file. The field derivatives or momenta follow the fields, in the same order.

For example, in the double quadratic model the fields are ϕ and χ , with ϕ being declared before χ in the description file (see §3.5). To plot only the components $\Sigma_{\phi\phi}$ and $\Sigma_{\chi\chi}$ we could use the selector

```
1 vis_toolkit::index_selector<2>().none().set_on( {0,0} ).set_on( {1,1} )
```

On the other hand, to plot components *except* the momentum cross-terms $\Sigma_{p_\phi p_\chi}$ and $\Sigma_{p_\chi p_\phi}$ we could use

```
1 vis_toolkit::index_selector<2>().all().set_off( {2,3} ).set_off( {3,2} )
```

7.6 Examples: double quadratic inflation

To illustrate the use of these derived quantities, consider generating plots for a set of standard observables in the double-quadratic model. We will use the following standard queries to select time- and wavenumber-configuration samples:

```
1 // time query -- all sample points
2 vis_toolkit::SQL_time_query all_times("1=1");
3
4 // time query -- last time
5 vis_toolkit::SQL_time_query last_time("serial IN (SELECT MAX(serial) FROM time_samples)");
6
7 // twopf query -- all configurations
8 vis_toolkit::SQL_twopf_query all_twopfs("1=1");
9
10 // threepf query -- all equilateral configurations
11 vis_toolkit::SQL_threepf_query all_equilateral("ABS(alpha) < 1E-5 AND ABS(beta-1.0/3.0) < 1E-5");
12
13 // threepf query -- isosceles triangles
14 vis_toolkit::SQL_threepf_query all_isosceles("ABS(alpha) < 1E-5");
15
16 // threepf query -- largest and smallest equilateral triangles
17 vis_toolkit::SQL_threepf_query large_small_equilateral("ABS(alpha) < 1E-5 AND ABS(beta-1.0/3.0) <
  ↪ 1E-5 AND wavenumber1 IN (SELECT MAX(serial) FROM twopf_samples UNION SELECT MIN(serial) FROM
  ↪ twopf_samples)");
```

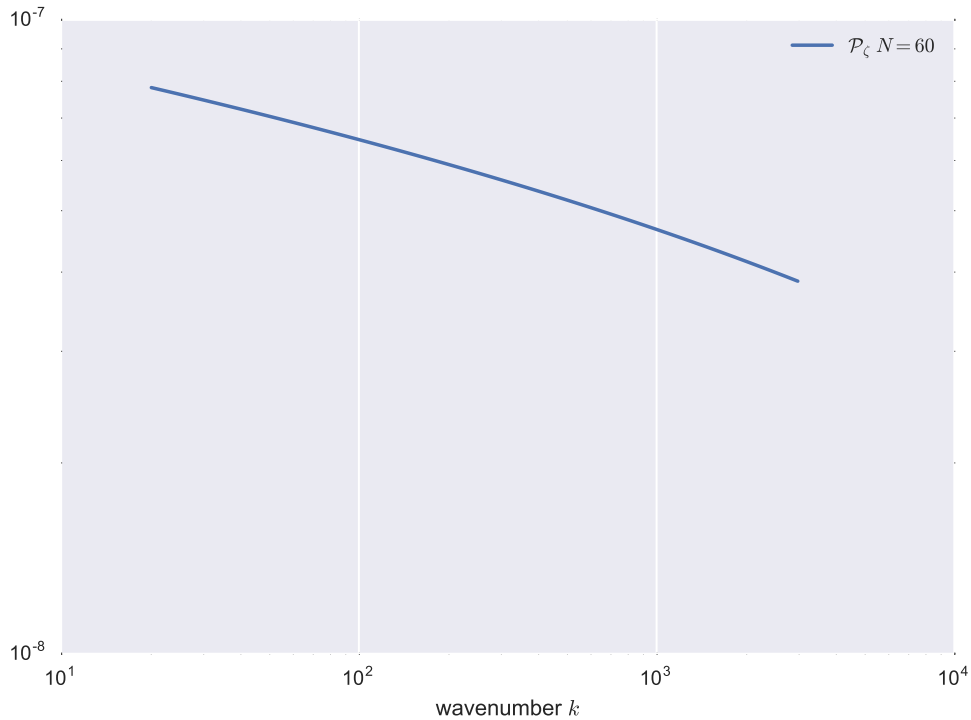


Figure 16. ζ 2-point function

7.6.1 ζ power spectrum

```

1 // 2. Zeta power spectrum
2
3 vis_toolkit::zeta_twopf_wavenumber_series<> zeta_twopf(ztk3, last_time, all_twopfs);
4 zeta_twopf.set_dimensionless(true);
5
6 vis_toolkit::wavenumber_series_plot<> zeta_twopf_plot("dquad.product.zeta-twopf.plot",
7   ↪ "twopf-plot.pdf");
8 zeta_twopf_plot.set_log_x(true);
9 zeta_twopf_plot += zeta_twopf;

```

This produces the plot of Fig. 16.

7.6.2 Spectral index for ζ power spectrum

```

1 // 3. Zeta power spectrum spectral index
2
3 vis_toolkit::zeta_twopf_wavenumber_series<> zeta_twopf_index(ztk3, last_time, all_twopfs);
4 zeta_twopf_index.set_dimensionless(true);
5 zeta_twopf_index.set_spectral_index(true);
6
7 vis_toolkit::wavenumber_series_plot<>
8   ↪ zeta_twopf_index_plot("dquad.product.zeta-twopf.index-plot", "twopf-index-plot.pdf");
9 zeta_twopf_index_plot.set_log_x(true);
10 zeta_twopf_index_plot += zeta_twopf_index;

```

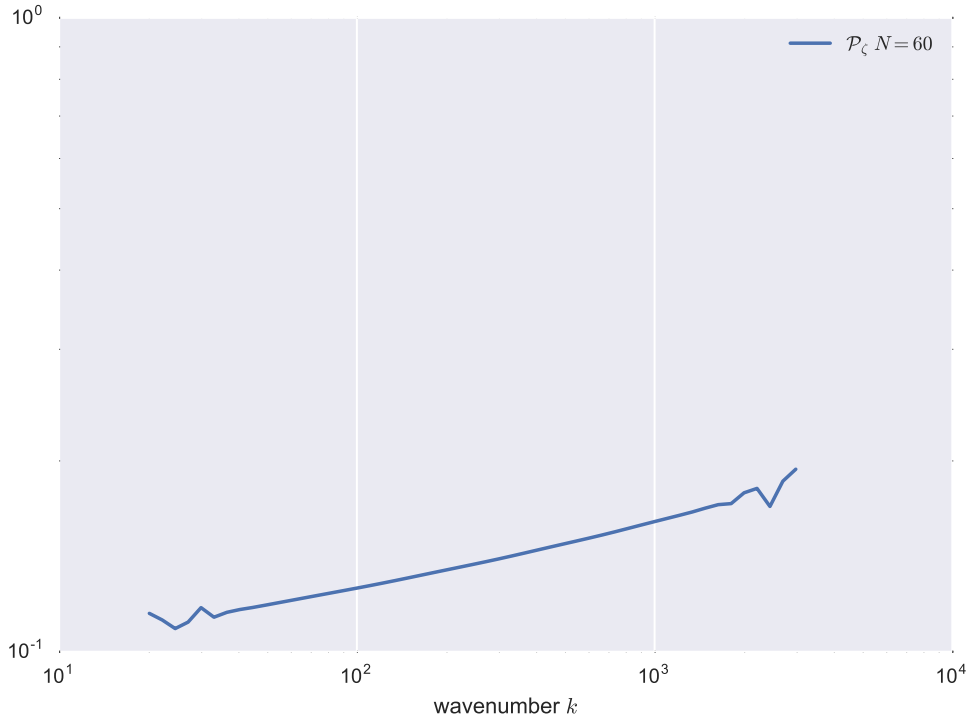



Figure 17. Spectral index of ζ two-point function

This produces the plot of Fig. 17. Notice the jitter near the ends of the line; see the discussion of spectral index calculations in §7.4.5. The results could be improved by extending the range of wavenumbers being sampled, to move these edge effects away from the region of interest.

7.6.3 Reduced bispectrum on equilateral configurations

```

1 // 4. Reduced bispectrum on equilateral configurations
2
3 vis_toolkit::zeta_reduced_bispectrum_wavenumber_series<> zeta_redbsp_equi(ztk3, last_time,
  ↪ all_equilateral);
4 zeta_redbsp_equi.set_current_x_axis_value(vis_toolkit::axis_value::k);
5
6 vis_toolkit::wavenumber_series_plot<>
  ↪ zeta_redbsp_equi_plot("dquad.product.zeta-redbsp.equi-plot", "equi-plot.pdf");
7 zeta_redbsp_equi_plot.set_log_x(true);
8 zeta_redbsp_equi_plot += zeta_redbsp_equi;

```

This produces the plot of Fig. 18. Notice the slight oscillations caused by settling of the heavy field into its minimum.

7.6.4 Spectral index of reduced bispectrum on equilateral configurations

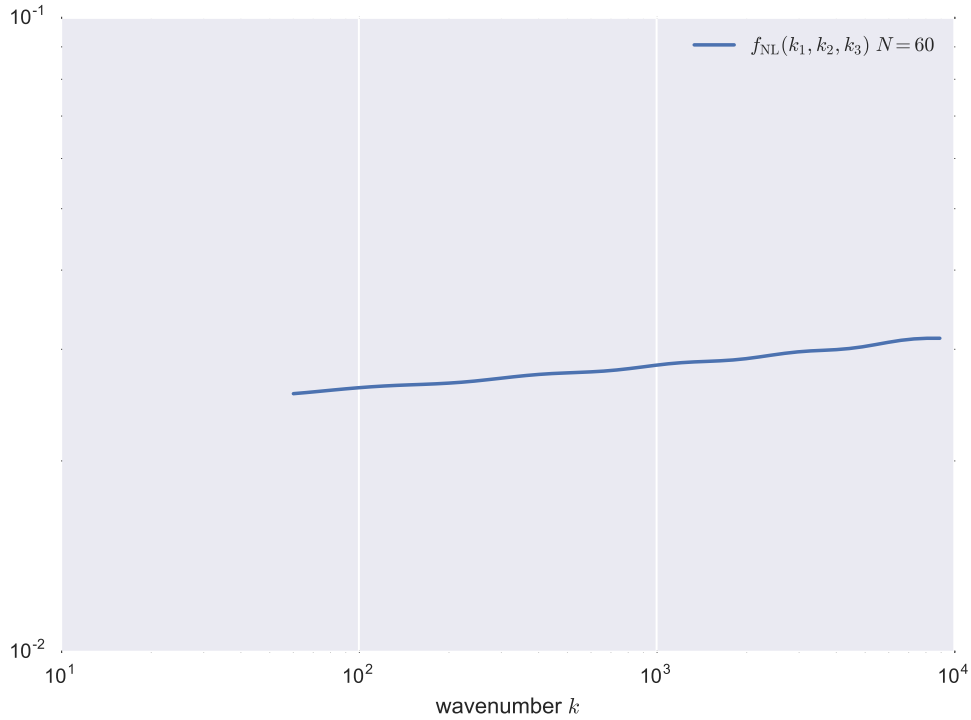


Figure 18. Reduced bispectrum on equilateral configurations of varying scale k_t

```

1 // 5. Spectral index of reduced bispectrum on equilateral configurations
2
3 vis_toolkit::zeta_reduced_bispectrum_wavenumber_series<> zeta_redbsp_equi_index(ztk3, last_time,
  ↪ all_equilateral);
4 zeta_redbsp_equi_index.set_spectral_index(true).set_current_x_axis_value(vis_toolkit::axis_value::k);
5
6 vis_toolkit::wavenumber_series_plot<>
  ↪ zeta_redbsp_equi_index_plot("dquad.product.zeta-redbsp.equi-index-plot", "equi-index.pdf");
7 zeta_redbsp_equi_index_plot.set_log_x(true);
8 zeta_redbsp_equi_index_plot += zeta_redbsp_equi_index;

```

This produces the plot of Fig. 19. The oscillatory structure is much more visible than it is in the amplitude. In general, obtaining accurate spectral indices requires higher accuracy in the integration. This can be achieved by increasing the number of e-folds of massless evolution, and by decreasing the absolute and relative tolerances if needed.

7.6.5 Squeezing dependence of reduced bispectrum: isosceles triangles

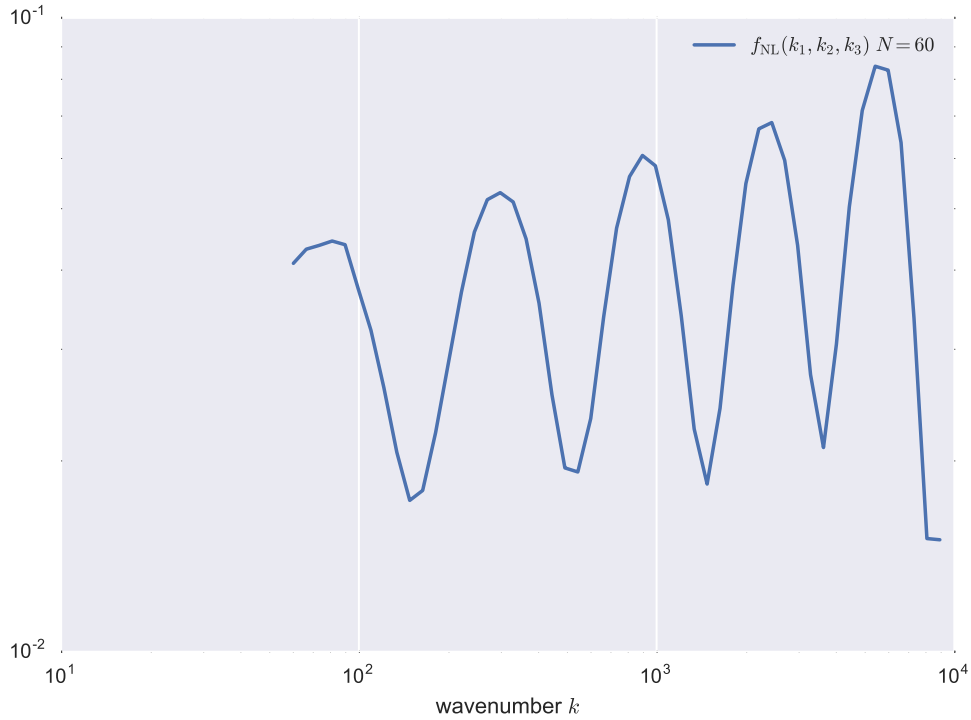


Figure 19. Spectral index (with k_t) of reduced bispectrum on equilateral configurations

```

1 // 6. Reduced bispectrum as a function of squeezing on isosceles triangles
2
3 vis_toolkit::zeta_reduced_bispectrum_wavenumber_series<> zeta_redbsp_squeeze(ztk3, last_time,
  ↪ all_isosceles);
4 zeta_redbsp_squeeze.set_current_x_axis_value(vis_toolkit::axis_value::squeeze_k3);
5
6 vis_toolkit::wavenumber_series_plot<>
  ↪ zeta_redbsp_squeeze_plot("dquad.product.zeta_redbsp.squeeze-plot", "squeeze-plot.pdf");
7 zeta_redbsp_squeeze_plot.set_log_x(true);
8 zeta_redbsp_squeeze_plot += zeta_redbsp_squeeze;

```

This produces the plot of Fig. 20. The general trend is clear, but there are obvious jumps in amplitude from configuration to configuration. This happens because the plot is constructed from a cubic mesh. Although only the squeezing ratio k_3/k_t is plotted on the x -axis, the configurations are also varying in k_t . To get a smooth line—for example, suitable for computing a spectral index—it would be necessary to switch to an $\alpha\beta$ -type mesh that would allow sampling from different values of k_3/k_t at fixed k_t .

7.6.6 Time evolution of 3pf correlation functions

The most commonly used data products are functions of wavenumber (or other configuration variables) at fixed time. Often this fixed time will be the end of inflation, although it may be earlier if the system converges to an adiabatic limit characterized by conservation of ζ (as it does for the double quadratic model).

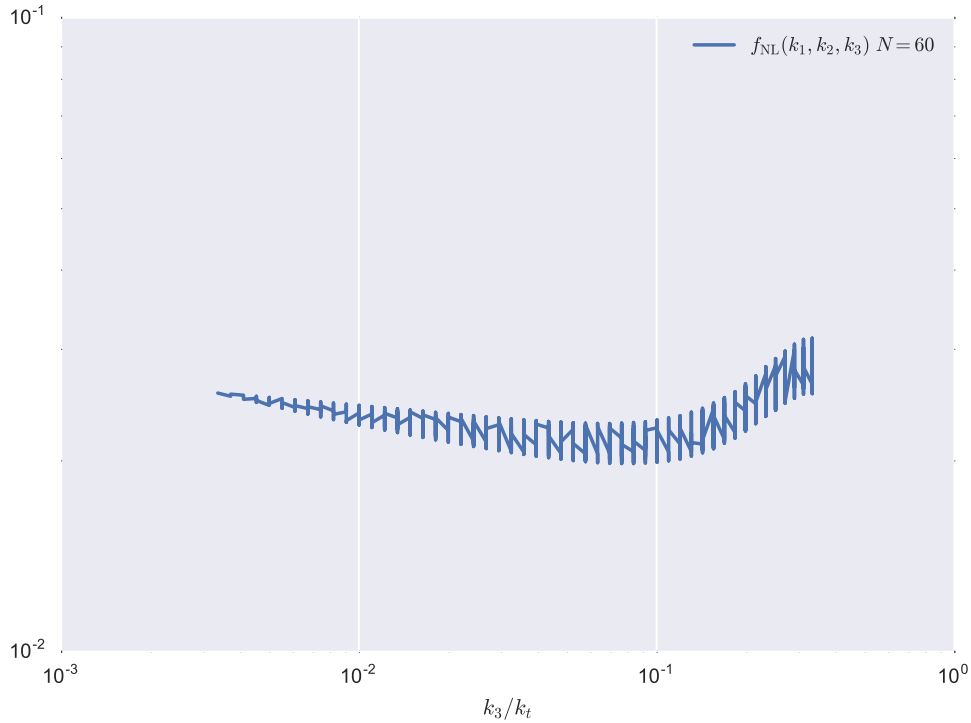


Figure 20. Variation of reduced bispectrum with squeezing k_3/k_t

However, it is also useful to plot the time *evolution* of individual quantities. This is especially useful to check for any anomalies in the integration that might make the final data products inaccurate. As a sanity check, it is useful to plot the evolution of the raw 3-point functions for at least a few scales.

```

1 // 7. Time evolution of some sample 3-point correlation functions
2
3 vis_toolkit::threepf_time_series<> threepf_time(tk3,
4   ↪ vis_toolkit::index_selector<3>(num_fields).none().set_on({ 0, 0, 0 }).set_on({ 1, 1, 1 }),
5   ↪ all_times, large_small_equilateral);
6
7 vis_toolkit::time_series_plot<> threepf_time_plot("dquad.product.threepf-time",
8   ↪ "threepf-time.pdf");
9 threepf_time_plot += threepf_time;

```

The resulting plot is shown in Fig. 21. Notice the use of ‘tags’ giving the k_t value, which distinguish between the different lines generated by the wavenumber configuration query; see the discussion of label tagging in §7.4.1.

Such plots are an especially useful diagnostic tool where they include the subhorizon evolution, here visible as a steeply falling straight line at the left-hand edge of the plot for the lines with $k_t = 8.94 \times 10^3$. In this region the individual wavefunctions oscillate rapidly but the *correlation function* is smooth, as was explained in the discussion of adaptive initial conditions in §5.1. In the absence of special features, the subhorizon evolution should be a smooth decaying power law. Any noise in these lines, or the appearance of oscillations,

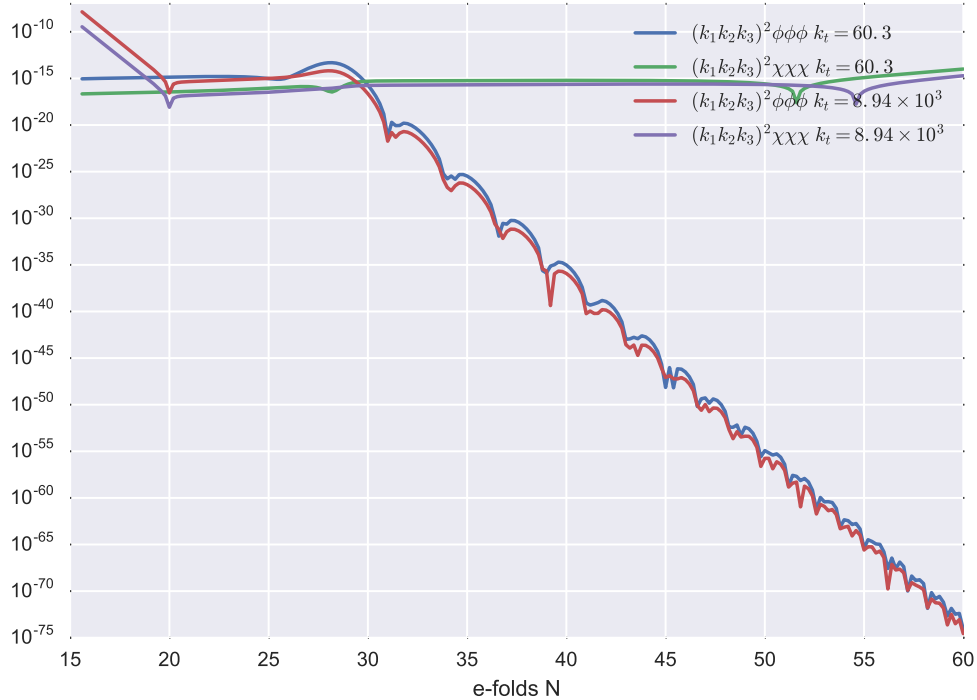


Figure 21. Time evolution of the 3-point functions $\langle \phi\phi\phi \rangle$ and $\langle \chi\chi\chi \rangle$ for the largest and smallest values of k_t

tends to indicate loss of accuracy during the integration. The normal response should be to tighten the numerical tolerances (§3.3), increase the number of e-folds of massless evolution (§4.3 and p.68), or both.

7.6.7 f_{NL} amplitude

Finally, consider setting up a plot of the amplitudes generated by inner-products with the equilateral, orthogonal and local templates. We can collect these in a separate function; see Fig. 22. The resulting plot is shown in Fig. 23 and can be compared with the hand-generated version Fig. 12.

8 Managing repositories

8.1 Managing records

§6.2 explained the system of ‘tags’ used to control which content groups are selected as data sources for postintegration or output tags. Tags can be set immediately, when each content group is generated, but it is also possible to adjust them after the group has been entered in the repository.

In addition to tags, CppTransport provides a facility to attach longer ‘notes’ to each group. These consist of free-format text and can be used for any purpose. For example, they

```

1 void write_fNL_products(transport::repository<>& repo, transport::initial_conditions<>& ics,
2                       transport::range<>& ts, transport::range<>& ks)
3 {
4     transport::threepf_cubic_task<> tk("dquad.threepf-linear", ics, ts, ks);
5     tk.set_adaptive_ics_efolds(5.0);
6     tk.set_description("Compute time history of the 3-point function on a linear grid");
7
8     transport::zeta_threepf_task<> ztk("dquad.threepf-linear-zeta", tk);
9     ztk.set_description(
10 ↪ "Convert the output from dquad.threepf-linear into zeta 2 and 3-point functions");
11
12     transport::fNL_task<> fNL_local("dquad.fNL-local", ztk,
13 ↪ vis_toolkit::bispectrum_template::local);
14     fNL_local.set_description(
15 ↪ "Compute inner product of double-quadratic bispectrum with local template");
16
17     transport::fNL_task<> fNL_equi("dquad.fNL-equi", ztk,
18 ↪ vis_toolkit::bispectrum_template::equilateral);
19     fNL_equi.set_description(
20 ↪ "Compute inner product of double-quadratic bispectrum with equilateral template");
21
22     transport::fNL_task<> fNL_ortho("dquad.fNL-ortho", ztk,
23 ↪ vis_toolkit::bispectrum_template::orthogonal);
24     fNL_ortho.set_description(
25 ↪ "Compute inner product of double-quadratic bispectrum with orthogonal template");
26
27     vis_toolkit::SQL_time_query all_times("1=1");
28
29     vis_toolkit::fNL_time_series<> local(fNL_local, all_times);
30     vis_toolkit::fNL_time_series<> equi(fNL_equi, all_times);
31     vis_toolkit::fNL_time_series<> ortho(fNL_ortho, all_times);
32
33     vis_toolkit::time_series_plot<> fNL_plot("dquad.product.fNL_plot", "fNL_plot.pdf");
34     fNL_plot.set_log_y(false).set_abs_y(false);
35     fNL_plot += local + equi + ortho;
36
37     transport::output_task<> out_tk("dquad.output.fNL");
38     out_tk += fNL_plot;
39
40     repo.commit(out_tk);
41 }

```

Figure 22. Function to generate f_{NL} tasks and derived products

could be used to add persistent working notes to an ongoing project, to highlight features when circulating data to collaborators, or to provide enriched documentation for archival purposes.

Finally, it is sometimes desirable to remove unneeded content groups from a repository. Notice, however, that `CppTransport` does *not* offer an option to remove or edit the details of initial conditions packages, tasks, or derived products. This is an intentional design choice. These details form part of the documentation associated with each content group, and if they were to be changed then some of this documentation would be lost or become ambiguous. If it is necessary to make adjustments to any of these definitions, it is preferable to add a new definition with a different name or to write into a new repository.

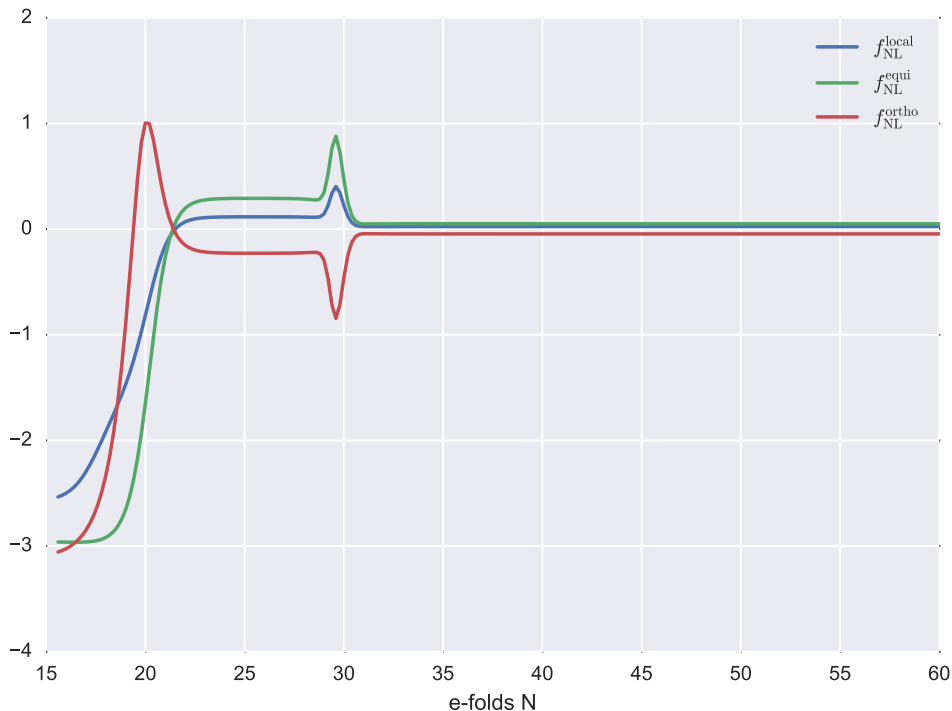


Figure 23. Time evolution of inner-product amplitudes $f_{\text{NL}}^{\text{local}}$, $f_{\text{NL}}^{\text{equi}}$ and $f_{\text{NL}}^{\text{ortho}}$. As above, we caution that these quantities must be interpreted with care and are not necessarily related to the constraints reported from experiment.

8.1.1 Specifying which objects to modify

CppTransport allows modifications to be applied to many different repository records simultaneously. To specify records use the `--object` command-line argument, followed by the name of a content group. It is possible to use multiple `--object` arguments to specify multiple records.

Alternatively, to name provided to `--object` can be enclosed in braces `{ ... }`. CppTransport will interpret the name between the braces as a regular expression and attempt to match it to any available content groups. For example, to match any content group produced in 2016 we could write `--object {2016.*}`.

8.1.2 Adding and removing tags

Adding tags is accomplished using the `--add-tag` command-line switch, followed by the name of a tag. If that tag contains spaces then it should be wrapped in quotation marks. The given tag is added to all content groups that match an argument provided to `--object`. To remove a tag from all such groups use `--delete-tag`.

8.1.3 Adding and removing notes

To add notes, use `--add-note` followed by the text to be added. If it contains spaces, it should be wrapped in quotation marks. The note is added to all content groups matching an argument provided to `--object`.

To remove a note, obtain a list of notes attached to the content group of your choice using `--info`. Then use `--delete-note` followed by the number of the note to be removed.

Warning

Notice that the given note is removed from every content group that matches an argument provided to `--option`. If the note you intend to delete is not in the same position in every content group then you will need to carry out the removal in batches.

8.1.4 Deleting content groups

To delete an unwanted content group use `--delete`. CppTransport will not allow you to delete content groups that were used as data sources for other groups that remain in the repository, because this would disrupt its ability to provide a provenance for those groups.

8.1.5 Lock and unlock groups

Finally, groups can be *locked* to prevent modifications. To do this use the `--lock` switch. Locked groups cannot be altered or deleted until they are unlocked using `--unlock`.

8.2 Summary of command-line options

This section summarizes the command-line options recognized by CppTransport executables.

Housekeeping functions:

- `--help`
Display brief usage information and a list of all available options.
- `--version`
Show version of CppTransport used to build the model headers, and the version of the runtime system. These need not be the same, although CppTransport requires the runtime system to be at least as recent as the version used to build the headers.
- `--license`
Display licensing information.
- `--models`
Show list of models understood by this executable.
- `--no-colour` or `--no-color`
Do not produce colourized output. Normally CppTransport will detect whether the terminal in which it is running can support colour. However, if you are redirecting CppTransport's output to a file then you may wish to manually suppress the use of colour.

- **--include**, or abbreviate to **-I**
Adds the following path to the list of paths searched for resources. Currently, the only resources needed by `CppTransport` are those used by the HTML report generator.

Configuration options:

- **--verbose**, or abbreviate to **-v**
Display extra status and update messages.
- **--repo**, or abbreviate to **-r**
Should be followed by a path identifying the repository to be used. If the repository does not exist then new, blank repository is created.
- **--caches**
 - batch-cache**
 - datapipe-cache**
 Followed by a cache size in Mb. Sets the corresponding cache size (or both caches, if the option **--caches** is used). The *batching cache* is used to temporarily hold the data products from integration in memory before flushing them to disk; see §4.5. The *datapipe cache* stores data used to generate derived products. This normally requires database access, which can be time consuming on a slow filing system. Storing data in memory can give a significant performance boost if the same data is re-used.
- **--network-mode**
Disable use of the SQLite write-ahead log. Must be used if the repository is stored on a network filing system such as NFS or Lustre, but should otherwise be omitted.

Job specification:

- **--create**
Write records held by this executable into the repository (§4.4.2).
- **--task**
Followed by the name of task. Adds the named task to the list of work.
- **--tag**
Specify a tag to be attached to any content groups generated by this `CppTransport` job. For postintegration or output tasks, filters the available content groups to those that share the specified tag. Can be repeated multiple times to specify more than one tag.
- **--checkpoint**
Set the checkpoint interval, measured in minutes. Overrides any default checkpoints set by individual tasks.
- **--seed**
Seed jobs using the specified content group.

Repository actions:

- **--object**
Select objects to be modified. Regular expressions can be used between curly braces `{ ... }`.
- **--lock**
Lock repository records (preventing modification or deletion) for content groups matching the object specification list.
- **--unlock**
Unlock repository records matching the object specification list.
- **--add-tag**
Add the specified tag to content groups matching the object specification list. Can be repeated multiple times to add more than one tag.
- **--delete-tag**
Remove the specified tag from content groups matching the object specification list. Can be repeated to delete multiple tags.
- **--add-note**
Add the specified note (which should be quoted if it contains spaces) to any content groups matching the object specification list. Can be repeated to add multiple notes.
- **--delete-note**
Specifies a note to remove by number (check the repository record using **--info** to obtain a list of notes). Can be applied to multiple content groups, but will remove the same numbered note from each list.
- **--delete**
Remove content groups matching the object specification list, provided no other content groups depend on them.

Notice that operations can be chained. For example, **--unlock** and **--delete** can be specified at the same time, in which case unlocking is performed *before* deletion. The same applies to other operations such as adding or removing tags and notes. If **--lock** is specified then the record is locked only after all other operations have been processed.

Repository reporting and status:

- **--record**
Perform recovery on the repository; see §4.6.
- **--status**
Print brief report showing repository status. Includes available tasks and the number of content groups attached to each task, in addition to the details of any in-flight jobs.
- **--inflight**
Similar to **--status**, but shows details of in-flight jobs only.

- **--info**
Report on a specified repository record. Matches any objects whose names begin with the specified string, so it is not necessary to write the name out exactly. Alternatively, a regular expression can be provided by wrapping it in curly braces `{ ... }`.
- **--provenance**
Report on the provenance of a specified output content group. The provenance report shows all content groups that contributed to each derived product generated as part of the group. Name matching is as for **--info**.
- **--html**
Write a HTML-format report on the contents of the repository to the specified folder.

Plotting options:

- **--plot-style**, or abbreviate to **-p**
Select a plotting style. See the discussion in §2.5.
- **--mpl-backend**
Force CppTransport to use a specified Matplotlib backend. See the discussion in §2.5.

Journaling options:

- **--gantt**
Write a process Gantt chart, showing the activities of each process in a multiprocess MPI job, to the specified file. Any output format supported by Matplotlib may be used, selected by its extension. Alternatively the extension `.py` may be specified to obtain the Python script suitable for generating the plot.
- **--journal**
Write a (very detailed) JSON-format journal showing the MPI communication between workers. Mostly of value when debugging.

9 Acknowledgments

It is a pleasure to acknowledge a longstanding collaboration with Mafalda Dias, Jonathan Frazer and David Mulryne.

Development of CppTransport has been supported by an ERC grant:

- *Precision tests of the inflationary scenario*, funded by the European Research Council under the European Union’s Seventh Framework Programme (FP/2007–2013) and ERC Grant Agreement No. 308082.

In addition, some development of CppTransport has been supported by other funding sources. Portions of the work described in this document have been supported by:

- The UK Science and Technology Facilities Council via grants ST/I000976/1 and ST/L000652/1, which funded the science programme at the University of Sussex Astronomy Centre from April 2011–March 2014 and April 2014–March 2017, respectively.

- The Leverhulme Trust via a Philip Leverhulme Prize.
- The National Science Foundation Grant No. PHYS-1066293 and the hospitality of the Aspen Center for Physics.
- The hospitality of the Higgs Centre for Theoretical Physics at the University of Edinburgh, and the Centre for Astronomy & Particle Physics at the University of Nottingham.

A Third-party software used by CppTransport

The CppTransport sources incorporate portions of the following open source projects:

- The GinacPrint common subexpression elimination algorithm made available by Doug Baker.

<http://www.ginac.de/pipermail/ginac-list/2010-May/001631.html>

License: GPL-2

This is incorporated in the source files

```
translator/backends/infrastructure/language_concepts/cse.cpp
translator/backends/infrastructure/language_concepts/cse.h
```

The CppTransport translator and runtime system are linked to the following libraries. The build process assumes they are available on the system, but does not automatically install them.

The CppTransport sources do not include source code (or derivatives of the source code) from these libraries; they only link to them as external resources.

- GiNaC (used by translator)
 - <http://www.ginac.de>
 - License: GPL-2
- The Boost libraries (used by translator and runtime system)
 - <http://www.boost.org>
 - License: Boost Software License
- SQLite (used by runtime system)
 - <https://www.sqlite.org>
 - License: Public Domain (<https://www.sqlite.org/copyright.html>)
- OpenSSL (used by runtime system)
 - <https://www.openssl.org>
 - License: OpenSSL License (<https://www.openssl.org/source/license.html>)

In addition, the CppTransport build process automatically downloads and installs the following libraries. They are statically linked to executables constructed by (1) running the translator and (2) building the resulting code using the provided runtime system.

The CppTransport sources do not include source code (or derivatives of the source code) from these libraries. Compiled executables using the provided runtime system link to them only as external resources.

- SPLINTER
<https://github.com/bgrimstad/splinter>
License: Mozilla public license (see `thirdparty/License/SPLINTER.txt`)
- JsonCPP
<https://github.com/open-source-parsers/jsoncpp>
License: MIT License (see `thirdparty/License/JsonCpp.txt`)

CppTransport also depends on the Eigen library using the version bundled as part of SPLINTER.

- Eigen
http://eigen.tuxfamily.org/index.php?title=Main_Page
License: Mozilla public license (for details, see files installed by the SPLINTER build process)

Also, the CppTransport platform bundles parts of the following open source projects. These parts are included in the Git repository for CppTransport or the installation tarball in the `thirdparty/` directory.

The CppTransport sources do not include source code (or derivatives of the source code) from this projects. It depends on them only as external resources that are used by HTML reports.

- jQuery
<https://jquery.com/download/>
License: MIT License (see `thirdparty/License/jquery.txt`)
- Twitter Bootstrap
<http://getbootstrap.com>
License: MIT License (see `thirdparty/License/Bootstrap.txt`)
- bootstrap-tab-history
<http://mnarayan01.github.io/bootstrap-tab-history/>
License: Apache License (see `thirdparty/License/bootstrap-tab-history.txt`)
- DataTables
<https://datatables.net>
License: MIT License (see `thirdparty/License/DataTables.txt`)
- Prism.js
<http://prismjs.com>
License: MIT license (see `thirdparty/License/prism.txt`)

References

- [1] A. H. Guth, *The Inflationary Universe: A Possible Solution to the Horizon and Flatness Problems*, *Phys.Rev.* **D23** (1981) 347–356.
- [2] A. A. Starobinsky, *A New Type of Isotropic Cosmological Models Without Singularity*, *Phys.Lett.* **B91** (1980) 99–102.
- [3] A. Albrecht and P. J. Steinhardt, *Cosmology for Grand Unified Theories with Radiatively Induced Symmetry Breaking*, *Phys.Rev.Lett.* **48** (1982) 1220–1223.
- [4] S. Hawking and I. Moss, *Supercooled Phase Transitions in the Very Early Universe*, *Phys.Lett.* **B110** (1982) 35.
- [5] A. D. Linde, *A New Inflationary Universe Scenario: A Possible Solution of the Horizon, Flatness, Homogeneity, Isotropy and Primordial Monopole Problems*, *Phys.Lett.* **B108** (1982) 389–393.
- [6] A. D. Linde, *Chaotic Inflation*, *Phys.Lett.* **B129** (1983) 177–181.
- [7] M. Dias, R. H. Ribeiro, and D. Seery, *The δN formula is the dynamical renormalization group*, [1210.7800](#).
- [8] A. J. Tolley and M. Wyman, *The Gelaton Scenario: Equilateral non-Gaussianity from multi-field dynamics*, *Phys. Rev.* **D81** (2010) 043502, [[0910.1853](#)].
- [9] X. Chen and Y. Wang, *Large non-Gaussianities with Intermediate Shapes from Quasi-Single Field Inflation*, *Phys. Rev.* **D81** (2010) 063511, [[0909.0496](#)].
- [10] X. Chen and Y. Wang, *Quasi-Single Field Inflation and Non-Gaussianities*, *JCAP* **1004** (2010) 027, [[0911.3380](#)].
- [11] X. Chen and Y. Wang, *Quasi-Single Field Inflation with Large Mass*, *JCAP* **1209** (2012) 021, [[1205.0160](#)].
- [12] Z. Kenton and D. J. Mulryne, *The squeezed limit of the bispectrum in multi-field inflation*, *JCAP* **1510** (2015), no. 10 018, [[1507.08629](#)].
- [13] A. Pukhov, E. Boos, M. Dubinin, V. Edneral, V. Ilyin, D. Kovalenko, A. Kryukov, V. Savrin, S. Shichanin, and A. Semenov, *CompHEP: A Package for evaluation of Feynman diagrams and integration over multiparticle phase space*, [hep-ph/9908288](#).
- [14] **CompHEP** Collaboration, E. Boos, V. Bunichev, M. Dubinin, L. Dudko, V. Ilyin, A. Kryukov, V. Edneral, V. Savrin, A. Semenov, and A. Sherstnev, *CompHEP 4.4: Automatic computations from Lagrangians to events*, *Nucl. Instrum. Meth.* **A534** (2004) 250–259, [[hep-ph/0403113](#)].
- [15] A. Pukhov, *CalcHEP 2.3: MSSM, structure functions, event generation, batchs, and generation of matrix elements for other packages*, [hep-ph/0412191](#).
- [16] A. Belyaev, N. D. Christensen, and A. Pukhov, *CalcHEP 3.4 for collider physics within and beyond the Standard Model*, *Comput. Phys. Commun.* **184** (2013) 1729–1769, [[1207.6082](#)].
- [17] T. Hahn and M. Perez-Victoria, *Automatized one loop calculations in four-dimensions and D-dimensions*, *Comput. Phys. Commun.* **118** (1999) 153–165, [[hep-ph/9807565](#)].
- [18] T. Hahn, *Generating Feynman diagrams and amplitudes with FeynArts 3*, *Comput. Phys. Commun.* **140** (2001) 418–431, [[hep-ph/0012260](#)].
- [19] T. Hahn and M. Rauch, *News from FormCalc and LoopTools*, *Nucl. Phys. Proc. Suppl.* **157** (2006) 236–240, [[hep-ph/0601248](#)]. [[236\(2006\)](#)].
- [20] S. Agrawal, T. Hahn, and E. Mirabella, *FormCalc 7*, *J. Phys. Conf. Ser.* **368** (2012) 012054,

[1112.0124].

- [21] A. Kanaki and C. G. Papadopoulos, *HELAC: A Package to compute electroweak helicity amplitudes*, *Comput. Phys. Commun.* **132** (2000) 306–315, [[hep-ph/0002082](#)].
- [22] A. Cafarella, C. G. Papadopoulos, and M. Worek, *Helac-Phegas: A Generator for all parton level processes*, *Comput. Phys. Commun.* **180** (2009) 1941–1955, [[0710.2427](#)].
- [23] F. Maltoni and T. Stelzer, *MadEvent: Automatic event generation with MadGraph*, *JHEP* **02** (2003) 027, [[hep-ph/0208156](#)].
- [24] J. Alwall, P. Demin, S. de Visscher, R. Frederix, M. Herquet, F. Maltoni, T. Plehn, D. L. Rainwater, and T. Stelzer, *MadGraph/MadEvent v4: The New Web Generation*, *JHEP* **09** (2007) 028, [[0706.2334](#)].
- [25] J. Alwall, M. Herquet, F. Maltoni, O. Mattelaer, and T. Stelzer, *MadGraph 5 : Going Beyond*, *JHEP* **06** (2011) 128, [[1106.0522](#)].
- [26] J. Alwall, R. Frederix, S. Frixione, V. Hirschi, F. Maltoni, O. Mattelaer, H. S. Shao, T. Stelzer, P. Torrielli, and M. Zaro, *The automated computation of tree-level and next-to-leading order differential cross sections, and their matching to parton shower simulations*, *JHEP* **07** (2014) 079, [[1405.0301](#)].
- [27] T. Gleisberg, S. Hoeche, F. Krauss, A. Schalicke, S. Schumann, and J.-C. Winter, *SHERPA 1. alpha: A Proof of concept version*, *JHEP* **02** (2004) 056, [[hep-ph/0311263](#)].
- [28] T. Gleisberg, S. Hoeche, F. Krauss, M. Schonherr, S. Schumann, F. Siegert, and J. Winter, *Event generation with SHERPA 1.1*, *JHEP* **02** (2009) 007, [[0811.4622](#)].
- [29] M. Moretti, T. Ohl, and J. Reuter, *O’Mega: An Optimizing matrix element generator*, [[hep-ph/0102195](#)].
- [30] W. Kilian, T. Ohl, and J. Reuter, *WHIZARD: Simulating Multi-Particle Processes at LHC and ILC*, *Eur. Phys. J.* **C71** (2011) 1742, [[0708.4233](#)].
- [31] M. A. Dobbs *et al.*, *Les Houches guidebook to Monte Carlo generators for hadron collider physics*, in *Physics at TeV colliders. Proceedings, Workshop, Les Houches, France, May 26-June 3, 2003*, pp. 411–459, 2004. [[hep-ph/0403045](#)].
- [32] C. Ringeval, P. Brax, C. van de Bruck, and A.-C. Davis, *Boundary inflation and the WMAP data*, *Phys.Rev.* **D73** (2006) 064035, [[astro-ph/0509727](#)].
- [33] J. Martin and C. Ringeval, *Inflation after WMAP3: Confronting the Slow-Roll and Exact Power Spectra to CMB Data*, *JCAP* **0608** (2006) 009, [[astro-ph/0605367](#)].
- [34] C. Ringeval, *The exact numerical treatment of inflationary models*, *Lect.Notes Phys.* **738** (2008) 243–273, [[astro-ph/0703486](#)].
- [35] M. J. Mortonson, H. V. Peiris, and R. Easther, *Bayesian Analysis of Inflation: Parameter Estimation for Single Field Models*, *Phys.Rev.* **D83** (2011) 043505, [[1007.4205](#)].
- [36] R. Easther and H. V. Peiris, *Bayesian Analysis of Inflation II: Model Selection and Constraints on Reheating*, *Phys.Rev.* **D85** (2012) 103533, [[1112.0326](#)].
- [37] J. Norena, C. Wagner, L. Verde, H. V. Peiris, and R. Easther, *Bayesian Analysis of Inflation III: Slow Roll Reconstruction Using Model Selection*, *Phys.Rev.* **D86** (2012) 023505, [[1202.0304](#)].
- [38] L. C. Price, J. Frazer, J. Xu, H. V. Peiris, and R. Easther, *MultiModeCode: An efficient numerical solver for multifield inflation*, *JCAP* **03** (2015) 005, [[1410.0685](#)].
- [39] I. Huston and K. A. Malik, *Numerical calculation of second order perturbations*, *JCAP* **0909**

- (2009) 019, [[0907.2917](#)].
- [40] I. Huston and K. A. Malik, *Second Order Perturbations During Inflation Beyond Slow-roll*, *JCAP* **1110** (2011) 029, [[1103.0912](#)].
- [41] I. Huston and A. J. Christopherson, *Calculating Non-adiabatic Pressure Perturbations during Multi-field Inflation*, *Phys.Rev.* **D85** (2012) 063507, [[1111.6919](#)].
- [42] D. K. Hazra, L. Sriramkumar, and J. Martin, *On the discriminating power of f_{NL}* , [1201.0926](#).
- [43] V. Sreenath, D. K. Hazra, and L. Sriramkumar, *On the scalar consistency relation away from slow roll*, *JCAP* **1502** (2015), no. 02 029, [[1410.0252](#)].
- [44] M. Dias, J. Frazer, D. Mulryne, and D. Seery, “Numerical evaluation of the bispectrum in multiple-field inflation.” To appear, 2016.
- [45] K. Ahnert and M. Mulansky, *Odeint – Solving Ordinary Differential Equations in C++*, in *American Institute of Physics Conference Series* (T. E. Simos, G. Psihoyios, C. Tsitouras, and Z. Anastassi, eds.), vol. 1389 of *American Institute of Physics Conference Series*, pp. 1586–1589, Sept., 2011. [1110.3397](#).
- [46] G. I. Rigopoulos, E. P. S. Shellard, and B. J. W. van Tent, *Non-linear perturbations in multiple-field inflation*, *Phys.Rev.* **D73** (2006) 083521, [[astro-ph/0504508](#)].
- [47] G. Rigopoulos, E. Shellard, and B. van Tent, *Quantitative bispectra from multifield inflation*, *Phys.Rev.* **D76** (2007) 083512, [[astro-ph/0511041](#)].
- [48] F. Vernizzi and D. Wands, *Non-gaussianities in two-field inflation*, *JCAP* **0605** (2006) 019, [[astro-ph/0603799](#)].
- [49] D. J. Mulryne, D. Seery, and D. Wesley, *Moment transport equations for non-Gaussianity*, *JCAP* **1001** (2010) 024, [[0909.2256](#)].
- [50] D. J. Mulryne, D. Seery, and D. Wesley, *Moment transport equations for the primordial curvature perturbation*, *JCAP* **1104** (2011) 030, [[1008.3159](#)].
- [51] X. Gao, D. Langlois, and S. Mizuno, *Influence of heavy modes on perturbations in multiple field inflation*, *JCAP* **1210** (2012) 040, [[1205.5275](#)].
- [52] J. Elliston, D. J. Mulryne, D. Seery, and R. Tavakol, *Evolution of f_{NL} to the adiabatic limit*, *JCAP* **1111** (2011) 005, [[1106.2153](#)].
- [53] J. R. Fergusson and E. P. S. Shellard, *Primordial non-Gaussianity and the CMB bispectrum*, *Phys. Rev.* **D76** (2007) 083523, [[astro-ph/0612713](#)].
- [54] M. Dias, J. Elliston, J. Frazer, D. Mulryne, and D. Seery, *The curvature perturbation at second order*, *JCAP* **1502** (2015), no. 02 040, [[1410.3491](#)].
- [55] C. T. Byrnes, D. Regan, D. Seery, and E. R. M. Tarrant, *The hemispherical asymmetry from a scale-dependent inflationary bispectrum*, [1511.03129](#).
- [56] D. Babich, P. Creminelli, and M. Zaldarriaga, *The Shape of non-Gaussianities*, *JCAP* **0408** (2004) 009, [[astro-ph/0405356](#)].
- [57] J. R. Fergusson, M. Liguori, and E. P. S. Shellard, *General CMB and Primordial Bispectrum Estimation I: Mode Expansion, Map-Making and Measures of f_{NL}* , *Phys. Rev.* **D82** (2010) 023502, [[0912.5516](#)].
- [58] P. Creminelli, A. Nicolis, L. Senatore, M. Tegmark, and M. Zaldarriaga, *Limits on non-gaussianities from wmap data*, *JCAP* **0605** (2006) 004, [[astro-ph/0509029](#)].
- [59] L. Senatore, K. M. Smith, and M. Zaldarriaga, *Non-Gaussianities in Single Field Inflation and their Optimal Limits from the WMAP 5-year Data*, *JCAP* **1001** (2010) 028, [[0905.3746](#)].