Scipp: Scientific data handling with labeled multi-dimensional arrays for C++ and Python

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Abstract. scipp is heavily inspired by the Python library xarray. It enriches raw NumPy-like multi-dimensional arrays of data by adding named dimensions and associated coordinates. Multiple arrays are combined into datasets. On top of this, scipp introduces (i) implicit handling of physical units, (ii) implicit propagation of uncertainties, (iii) support for histograms, i.e., bin-edge coordinate axes, which exceed the data’s dimension extent by one, and (iv) support for event data. In conjunction these features enable a more natural and more concise user experience. The combination of named dimensions, coordinates, and units helps to drastically reduce the risk for programming errors. The core of scipp is written in C++ to open opportunities for performance improvements that a Python-based solution would not allow for. On top of the C++ core, scipp’s Python components provide functionality for plotting and content representations, e.g., for use in Jupyter Notebooks. While none of scipp’s concepts in isolation is novel per-se, we are not aware of any project combining all of these aspects in a single coherent software package.

Keywords: Software, Python, C++, data-processing, multi-dimensional

1. Introduction

The scipp library [1, 2] presented here can be seen as a step that combines requirements, knowledge, and capabilities from two streams of software development that have run independently for the past decade.

One the one hand, modern, flexible, and powerful concepts and tools have evolved (and still are evolving) in the Python ecosystem. Prime examples are pandas [3], xarray [4], and Jupyter [5]. For example, xarray provides flexible data structures for multi-dimensional data with named dimensions, coordinates, and attributes. This “labeled” way of storing data supports a good user-experience for developers and significantly reduces the risk for certain classes of bugs and errors, ensuring that scientific results are correct.

One the other hand, the Mantid framework [6] brings event-data handling for neutron-scattering experiments with support for physical units, uncertainties, and histograms. It is used at and jointly developed by ISIS, SNS, ESS, and ILL, with additional users and contributions from other neutron sources. One of Mantid’s strong points is processing of time-of-flight neutron scattering data in event mode, i.e., every neutron detected is recorded as a timestamp and a position index. Over the years however, new requirements arose that are inconvenient to handle in the existing framework. Examples include: (a) Storage of and visualization of data depending on arbitrary additional parameters, in particular scans of sample-environment parameters such as a sample temperature. (b) Storage of and visualization of data not depending on time-of-flight (or derived dimensions), e.g., for monochromatic
beamlines at reactor sources or neutron-imaging techniques. (c) Uncertainties and units attached to all entities: both to data and (optionally) its coordinates. (d) Possibility to have multiple axes along the same dimension. (e) Exploration of opportunities for performance improvements such as more efficient data layouts, the use of single-precision, and alternative approaches to multi-threading and parallelization.

Mantid lacks the flexibility to support such requirements without resorting to workarounds and furthermore misses several other desirable features of xarray such as a modern, simple, and coherent Python interface or good interoperability with NumPy. With Mantid’s codebase exceeding 2 million lines of code, significant changes in this direction are not feasible since they invariably become large-scale and breaking. In turn, xarray currently lacks support for features that are essential for neutron scattering data reduction. In particular, the following are must-have features:

(1) Automatic handling of physical units.
(2) Automatic propagation of uncertainties.
(3) Support for histograms, i.e., bin-edge coordinate axes, which exceed the data’s dimension extent by one.
(4) Support for event data, an array of nested random-length lists.

We therefore chose to develop a new library, scipp, combining above must-have features with flexible labeled data structures à la xarray. We considered it infeasible to implement all our additional requirements as contributions to the Python library xarray. One of the main reasons is the central role event-data plays for us — with xarray being based on regular dense NumPy arrays this would have been a major challenge and would have posed unknown risks for performance. For a more detailed discussion on the reasoning see Sec. 4.4.1.

scipp’s core is written in C++ but scipp is intended to be used mainly through its Python bindings.

The remainder of the paper is organized as follows. Section 2 gives an overview of scipp’s data structures and operations, Sec. 3 covers development methodologies, the Python interface, and technical details of scipp’s architecture, and Sec. 4 discusses performance, limitations, and related work. We conclude in Sec. 5.

2. Scipp fundamentals

2.1. Data structures and operations

The central data structures in scipp are Variable, DataArray, and Dataset. Variables are the building block used for data arrays and datasets. Conceptually, a variable consists of:

values a multi-dimensional array of values
variances a (optional) multi-dimensional array of variances for the array values
dims a list of dimension labels for each axis of the array
unit a physical unit of the values in the array

In other words, a variable represents an array-valued physical quantity. Based on this abstraction, we implement basic element-wise operations such as addition, multiplication, or trigonometric functions. Such operations can propagate uncertainties and handle physical units, and operations produce an error if the units of the operands are incompatible. The dimension labels are used to implement safe slicing, safe broadcasting, and safe transposition, and operations produce an error if dimensions and/or array shapes are incompatible.

DataArray consists of a single variable representing data, alongside dictionaries of coordinates and attributes. Each of the coordinates and attributes are variables themselves. The coordinate dictionary provides a mapping from a key to the corresponding coordinate. Just like xarray, we distinguish dimension-coordinates with a key equal to the dimension of the coordinate, and non-dimension-coordinates with a key that is not part of the coordinate’s

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1 Etymology: Scientific C++ library → Sci++ → scipp.
2 The latter two are conceptually very similar to DataArray and Dataset in the xarray Python library.
Fig. 1. scipp’s auto-generated visualization of structure and content of a dataset. The dataset contains four data arrays named “a”, “b”, “c”, and “d” (yellow). “a” is a 3-D array with an associated array of variances (visualized as a second array behind the value array), “b” is 2-D with variances, “c” is 1-D, and “d” is a scalar (0-D). The three dimensions ‘x’, ‘y’, and ‘z’ each come with an associated coordinate (green). ‘y’ has an additional auxiliary coordinate named “labels” (blue). Finally, there is one scalar attribute named “attr” (red). When viewed in a Notebook or a web browser, tooltips provide further information such as physical units and array shapes.

$$\text{delta} = \text{data}['a'][x', 1:3] - \text{scipp}.\text{mean} (\text{data}['b'], 'z')$$

# see text (1) (2) (4-8) (4,5) (1) (3)

Fig. 2. Computation with scipp’s Python interface combining item access, slicing, function application, and binary operators. Based on the two inputs on the right-hand side the resulting delta is a data array with units, dimensions, and coordinates given by the result of the slicing and computation.

dimensions. Non-dimension-coordinates are essentially auxiliary labels for an axis. Finally, attributes are supported to store arbitrary other metadata. Based on this, we define operations between data arrays, one of the central concepts in scipp:

1. **Compare** coordinate and label values and their units.
2. **Operate** on the data.
3. Ignore attributes unless there is a unique way of preserving them.

That is, a mismatch of any of the coordinates will produce an error and data is not modified. Since data and coordinates are each internally variables, operations automatically handle physical units and propagation of uncertainties. Dataset provides a dictionary of data arrays with **aligned dimensions**. Essentially it can be seen as a data array with multiple data entries, each identified by a name string. Operations between datasets match data items based on their name string.

At first the apparent complexity of such higher-level data structures compared to, e.g., a plain NumPy ndarray, may be overwhelming for new users. Therefore, scipp supports programmatic generation of a visualization of its data containers, e.g., for a dataset as shown in Fig. 1. This greatly simplifies writing of easy-to-read documentation and helps illustrating inside Jupyter Notebooks for teaching purposes. Furthermore, it is convenient as a quick tool to inspect in-memory data in day-to-day use when working in a Jupyter Notebook.

Operations with scipp’s data structures frequently make use of slicing. Just like NumPy, a slice operation in scipp returns a view, i.e., no copy is made. Similarly, accessing an entry of a dataset returns a view that is equivalent to a data array, without making a copy. In both cases, views can be used to modify the content of the data container they are referencing. However, views prevent any modification that would break invariants of the data container. For example, a slice of a variable cannot be used to modify the unit of the variable, since this would require storing a different unit for different elements of the same variable. Similarly, a view of a data array cannot be used to change shape or dimension labels, since this would break the invariant of the dataset guaranteeing that dimensions of all data in the set are aligned.

Structuring information into the categories data, coordinates, and attributes and characterizing them with names, dimension names, and units is essentially a handle for controlling the behavior of operations. As an example,
Fig. 3. One-dimensional data array with event data (yellow), the raw data for a two-dimensional histogram. In addition to the coordinate for ‘x’ (green), there is an event coordinate (green) matching the length of the data. An event coordinate is always required if there is event data since by definition every data value is “measured” at a different coordinate value.

consider the line of code in Fig. 2 processing the dataset from Fig. 1. A Python user who has previously worked with NumPy will quickly be able to grasp the meaning and intention of this code, without much explanation: We select a data item from a dictionary-like object by its name, slice it along a certain dimension, and then subtract the mean along another dimension of a different data item. We break down what is happening under the hood to highlight the hidden power here:

1. Data items are selected by name (here: “a” and “b”).
2. Slice based on named dimension (here: slice “a” along ‘x’).
3. Apply other operation based on named dimension (here: mean along ‘z’).
4. Propagate uncertainties (here: mean and \(-\) (subtraction)).
5. Handle physical units (here: mean and \(-\) (subtraction)).
6. Match coordinates (here: \(-\) (subtraction)).
7. Broadcast into missing dimensions (here: \(-\) (subtraction)).
8. Transpose matching dimensions (not required here).

With the exception of (4) and (5) this is exactly what xarray also supports, unless event data is involved. For anyone familiar with NumPy, items (2), (3), (7), and (8) bring an immediate improvement since they avoid the need to keep track of and remember dimension order, to explicitly broadcast, and to explicitly transpose. Altogether, scipp’s data structures enable a brief and intuitive syntax that nevertheless handles all required concepts under the hood. With correctness of the programmatic operations built into the framework, users are free to focus on the intent when writing code for their scientific purposes.

2.2. Event data

Processing neutron-scattering data requires dealing with event data. Event data is a certain form of unaligned sparse data arising from recording the time-of-flight of every detected neutron alongside metadata such as a pixel identifier and an index of the proton pulse that produced the neutron. The data stored per neutron is tiny, typically between 1 and 4 integers or floating-point values, i.e., between 4 Byte and 32 Byte, depending on whether single-precision or double-precision is used. As an in-memory representation we commonly store a separate list of neutron events for every pixel. Structurally, event data amounts to an array of random-length lists — not to be confused with a sparse matrix or a sparse array which may represent a matrix with many “zero” entries in a packed format. In other words, the latter is aligned but sparse data, whereas event data is unaligned. This is essentially raw data for creating a histogram for every pixel, i.e., raw data for a 2-D (or higher) array.

Due to the importance of event data in the field, scipp is designed to support this particular form of sparse data as arrays with list-valued elements. Figure 3 is an example of a data array containing event lists. Internally scipp is using an array of vectors to store event data that supports:
3. Technical details and usage

3.1. Methodologies and distribution

scipp is open source, licensed under the GPLv3, and is currently developed by the European Spallation Source (ESS). It is hosted on GitHub (see https://github.com/scipp/scipp) and is developed using up-to-date practices such as code reviews, unit testing, and continuous integration. The released version 0.3.1 is for experimental use and not production-ready yet. We provide conda packages for easy installation and integration in existing Python environments.

scipp is implemented in C++. This choice gives maximum freedom in terms of performance optimization and will allow for interfacing with existing C++ applications like Mantid. The use of the recent C++17 revision of the standard played a central part in keeping the library flexible, small, and maintainable — despite its flexibility and number of features scipp is currently just 10,000 lines of code of C++, not counting unit tests and benchmarks. It is intended that most users would interface with scipp using its Python bindings, which are implemented using pybind11 [8]. On the Python side, scipp is designed to play nicely with NumPy. In particular, value and variance arrays in a variable can be initialized from NumPy arrays, and NumPy functions can be directly applied to those arrays. This allows for integration with a large variety of other scientific software.

Jupyter Notebooks are rapidly becoming a go-to solution for scientific data handling, combining advantages from scripting interfaces with those of a graphical user-interface. Therefore, in addition to visualizations as shown in Fig. [1] scipp also provides table-displays for 1-D data and easy-to-use plotting functionality for any number of dimensions based on Matplotlib [9]. Labeled dimensions, coordinates, physical units, and uncertainties stored in
a data array or dataset alongside data allow for direct creation of meaningful plots without the need for additional user-provided information. An example is given in Fig. 4. Most of scipp’s documentation (see https://scipp.github.io) is also written as Jupyter Notebooks and can thus be downloaded, interacted with, and experimented with to serve as a starting point for new users. The documentation also includes a number of tutorials in the form of Jupyter Notebooks, such as the one displayed in the next section.

During development of scipp we favor clean code over hypothetical performance gains. When we do implement concrete optimizations, we drive and justify this using benchmarks modeling real workloads.

3.2. Usage example

To give a better understanding of the mechanics of scipp and of its current capabilities, a concrete usage example is provided in Fig. 5. The depicted workflow uses scipp in a Jupyter Notebook to process neutron-scattering data. To avoid an abrupt loss of encapsulated features and know-how when switching from using Mantid to using scipp, conversion between the respective data containers is supported. In this case this happens internally in scipp.neutron.load, which is actually relying on Mantid to load NeXus [10] files. The resulting data array includes data and coordinates, as well as attributes holding the sample and run information, and a simplified instrument geometry.

3.3. Architecture

3.3.1. Type erasure

scipp’s Variable must support a considerable number of types — just our basic use cases include double, float, int64_t, int32_t, std::string, bool, DataArray for storing complex information such as neutron monitors, Eigen::Vector3d for positions in space, and event lists containing double, float, int64_t, and int32_t. In C++ this is obviously addressed using templates. However, since variables are combined in data arrays and datasets, a hypothetical templated class Variable would lead to a combinatoric explosion in the number of required template instantiations for the DataArray and Dataset classes. Once we also consider that operations between data arrays with different type content are required, it becomes clear that this problem is intractable.

To support storage of the various required types of data and combining arbitrary variables in data arrays or datasets, scipp thus employs type erasure [11]. That is, Variable is not a templated class, i.e., there is no Variable<double> and Variable<float>. The actual data type of the elements is not reflected in the class type but is erased by an internal mechanism based on concept-based polymorphism [12]. The result is a simple high-level C++ interface that feels similar to an interface in Python. This high-level interface can be used as long as the existing operations are sufficient as building blocks. When this is not the case a crucial difficulty with type-erasure becomes apparent: developers must either (a) choose the data type when implementing an operation and fail if the input does not have the expected type or (b) provide an implementation for all possible combinations of input types. The former is generally too limiting and contravenes the flexibility gained from generic data structures and type erasure. The next section describes how scipp facilitates the latter.

3.3.2. Generic transform algorithms

To leverage the power of type-erasure without excessive templating and specializations in implementations of operations, scipp employs a — to our knowledge — novel mechanism. One approach would be to implement all operations as virtual methods of the underlying VariableConcept used for type erasure. However, for operations with two (or more) inputs this would require double-dynamic (or multiple-dynamic) dispatch which is cumbersome to implement in C++, quickly leads to an intractable amount of code, and would make adding user-defined operations virtually infeasible. Our solution works as follows:

In this case only pixel positions are required, so the instrument geometry in scipp does not include pixel shapes or rotations.

While in practice only a limited subset of type combinations will be used, scipp is mainly used through its Python scripting interface, so we have to compile and build all possible type combinations into the library.

Including first and foremost a large number of built-in operations.
Imports for `scipp` and NumPy:

```python
import numpy as np
import scipp as sc
from scipp.plot import plot
```

Loading NeXus files:

```python
tof_sam = sc.neutron.load('PG3_4844_event.nxs')
tof_van = sc.neutron.load('PG3_4866_event.nxs')
```

Convert units to \(d\)-spacing (interplanar lattice spacing):

```python
sam = sc.neutron.convert(tof_sam, 'tof', 'd-spacing')
van = sc.neutron.convert(tof_van, 'tof', 'd-spacing')
```

Histogram event data:

```python
bins = sc.Variable(dims=['d-spacing'],
                   unit=sc.units.angstrom,
                   values=np.arange(0.3, 2.0, 0.001))
h = sc.Dataset({'sample':sc.histogram(sam, bins),
                 'vanadium':sc.histogram(van, bins)})
```

Create plot of counts depending on \(d\)-spacing and spectrum:

```python
plot(h['sample']['d-spacing',100:400])
```

Reduce data into a single spectrum using `scipp.sum`:

```python
summed = sc.sum(h, 'spectrum')
plot(summed)
```

Normalize sample data to vanadium:

```python
normalized = summed['sample'] / summed['vanadium']
plot(normalized)
```

Plots of quantities against time-of-flight or \(d\)-spacing and spectrum are often hard to read since “spectrum” is not a dimension with physical meaning but an instrument artifact. `scipp`’s `groupby` provides a convenient tool for converting “spectrum” to something more useful. We group and combine data based on scattering angle \(\theta\) using `groupby`:

```python
theta = sc.neutron.scattering_angle(tof_sam)
tof_sam.coords['theta'] = theta
theta_bins = sc.Variable(dims=['theta'],
                         unit=sc.units.rad,
                         values=np.linspace(0.5, 1.2, num=1000))
theta_tof_sample = sc.groupby(tof_sam, 'theta',
                              bins=theta_bins).flatten('spectrum')
```

Create plot depending on time-of-flight and \(\theta\), showing intensity peaks following a \(\sin\), as expected from Bragg’s law:

```python
plot(theta_tof_sample, bins={'tof':tof_bins})
```

Fig. 5. Example of `scipp`-usage in a Jupyter Notebook for a (simplified) data reduction workflow for time-of-flight powder-diffraction data in event mode. See the electronic version of the article for high-resolution figures.
Variable radius(const Variable &varX, const Variable &varY) {
    return transform<
tuple<double, double>, tuple<double, float>,
tuple<float, double>, tuple<float, float>>(
        varX, varY, [](const auto x, const auto y) {
            return sqrt(x * x + y * y);
        });
}

Fig. 6. Example of the internal transform function used to compute $\sqrt{a^2 + b^2}$. The call to transform requires as explicit template arguments a list of all type combinations of the input arguments varX and varY that are to be supported. In practice scipp has pre-defined sets of commonly used combinations, so this does not need to be spelled out explicitly in all cases. The third function argument of transform is a functor, in this case a lambda. transform iterates over the value arrays (and, if present, variance arrays) of the inputs, transposing and broadcasting if required, and applies the functor to all elements, including the case of elements with attached uncertainties. The unit is also transformed using the functor. Based on the input’s dimensions, transform automatically creates an output variable with the correct dimensions.

- Use C++17’s type-safe union type, std::variant, with alternative types VariableConceptT<T> for a selected set of types T. In practice this includes, e.g., double, float, int64_t, and int32_t, i.e., the set of known fundamental types that make up the majority of data.
- Store the additional alternative type VariableConcept to handle any other data types that are not built-in or known to the core library. This is a fallback and implies that data stored using this alternative cannot make use of the mechanism described next.
- Provide transform and transform_in_place algorithms (in the spirit of std::transform) that can apply arbitrary lambdas or functors to a set of input variables. An example is given in Fig. 6. Internally this is using a visitation approach as provided by std::visit to branch to the correct instantiation based on the alternative types of all the input’s respective underlying variants. In practice we cannot use std::visit due to the large combinatoric factor when considering all possible types of all inputs. Instead, transform requires a list of supported type combinations of inputs. This is then used to generate all required branches.

The crucial point here is the visitation approach, bypassing the C++ restriction preventing virtual methods from being templated, while the fallback alternative in the variant keeps the flexibility of storing arbitrary data. transform automatically handles units, propagation of uncertainties, dense and event data (including mixing the two), transposition, and broadcasting. Any operation implemented based on transform will automatically leverage all this functionality, and implicitly benefit from using a single unified implementation that is well tested. It is also used internally for implementing the majority of element-wise operations between variables.

4. Status and evaluation

4.1. Performance

At the time of writing scipp has not been optimized for performance in its entirety. In particular it is currently single-threaded. The current target application of scipp is data-reduction for neutron data. Ignoring I/O, the majority of these workloads is bound by memory-bandwidth when individual reduction steps are considered in isolation. This implies two things: (1) It is comparatively simple to optimize code such that it hits the bandwidth limit, as long as memory allocation is avoided. The majority of scipp’s basic operations are optimized to this

\[6\] Preliminary support for multi-threading based on Intel Threading Building Blocks has been added to scipp since the original version of this manuscript, but a detailed discussion is beyond the scope of this article and will be included in a future publication.
effect(2) To overcome this limit we must either move to multi-node parallelization, employ cache-blocking techniques to make better use of the CPU caches, or both.

Part of the motivation for work on scipp is to open the opportunity for experimentation and investigation of aspect (2) in more detail. Such investigations would be virtually impossible within the Mantid framework due to its size. The mentioned approaches each come with advantages and disadvantages as well as limitations which require a detailed analysis and prototyping. The decision is further complicated by the fact that hdf5-based I/O, which is the most common format in the community, has very limited support for multi-threading but could see potential speedups from multi-process parallelism. Specifically for data-reduction of neutron-scattering data, part of the remit of the scipp development is to attempt to push the envelope of what can be handled on a single-node system with multi-threading, despite ever-increasing data volumes. Multi-process and multi-node parallelization always add complexity — even with modern solutions such as dask — and it is often beneficial to avoid such parallelization if feasible.

4.2. Limitations and shortcomings

Every choice has its downsides and also scipp comes with a number of limitations that may or may not be significant, depending on the use case.

(a) scipp does currently not support native I/O. Instead, we leverage Mantid to load data from disk (or save it to disk), converting the loaded data into a data array or dataset after loading. This certainly comes with a performance penalty and native scipp I/O is likely to be implemented in the future, at least for file formats where performance is crucial.

(b) scipp’s current implementation of physical units is based on boost’s units library. The limitation here is that boost::units is a compile-time unit implementation, i.e., all possible (required) combinations of base units must be known at compile time and built into the library. For specific scientific applications like data reduction of neutron-scattering data it should be possible to provide an exhaustive list of all required units. In more general cases however scipp will just produce an error message until the required unit is added, which requires recompilation of the library. We hope that this is a temporary limitation until a suitable replacement of boost::units is available.

4.3. Developing data reduction workflows

One of the lessons learnt from Mantid is that algorithms are only useful if their contract is fulfilled, i.e., input data is expected to have certain dimensions, units, or metadata. scipp aims to overcome parts of — but by no means all of — these problems by relying on small and generic building blocks. This reduces the number of preconditions and the contract is easier to fulfil. By comparison, Mantid has a significant number of algorithms that do multiple things or attempt to keep their contract flexible by supporting a variety of inputs. Over the years, additional special cases have been added to some of the existing algorithms. As a consequence, contracts for a variety of algorithms have become large and unclear, and in many cases developers need to consult the C++ implementation directly to understand limitations. The difference between the two approaches is best illustrated by an example:

(a) Mantid’s DiffractionFocussing is a specialized algorithm for powder reduction. It supports two ways to provide grouping information, one of which involves loading a file. Grouping is internally processed by specialized code. Data in input workspaces may be event data or histogrammed data. Processing can preserve events, or histogram the data on-the-fly. If the input is histogrammed data the algorithm furthermore rebins data to a common grid.

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7 Since there is no multi-threading yet this is the single-thread (or single-core) bandwidth, which is typically lower than the maximum bandwidth the whole CPU or multi-socket system can sustain. That being said, a single thread in a system with N cores can typically utilize significantly more than 1/N of the total bandwidth. We can conjecture that when multi-threading is introduced the existing optimizations would still support bandwidth-bound operation, provided that the workload is large enough to support efficient multi-threading.

8 dividing data into small chunks that fit into, e.g., L2 or L3 caches and applying a series of operations before proceeding with the next chunk
(b) scipp’s approach is the opposite. It turns out that the algorithm does not contain a single neutron-scattering specific step. Instead we use several independent steps to achieve the equivalent: (1) grouping information is loaded from files, (2) grouping information is preprocessed using `groupby`\(^9\) (3) data is reduced using generic `sum` (for histogrammed data) or `flatten` (for event data) operations, using `groupby` if multiple output spectra are required, and (4) histogram explicitly if desired.

Each of the components in scipp’s way of implementing the workflow has a low complexity and a low number of conditions in their contract. As a side benefit scipp’s approach also enables easier and more thorough unit testing and increases overall maintainability.

The part that scipp cannot overcome is obviously that the overall complexity of the task it is used for will not simply disappear. In the example above, at some point someone will need to write the code to execute steps (1-4). scipp’s goal is to make that easier by providing small and generic but powerful building blocks. This should give developers the opportunity to, e.g., choose to tailor workflows to a specific instrument without the need for complex algorithms supporting many cases, but at the same time avoiding large amounts of near-duplicate code. It is too early to tell how well this will work out in practice, and the choice between specialized but complex higher-level algorithms and, e.g., instrument-specific workflows will need to be made on a case-by-case basis.

Lastly, as a side effect of being generic, a “schema” or “standard” needs to be followed when organizing data and metadata in a data array or dataset. For example, neutron-specific algorithms like unit conversion will expect certain metadata in particular places, and will simply fail if this contract is violated. In practice we essentially define this as part of our file loaders or converters from Mantid. This is not very different from Mantid where despite fixed structures information may still be missing, e.g., missing instrument information such as the position of the sample will lead to a failure in ConvertUnits, i.e., scipp’s generality is not necessarily introducing a new problem.

4.4. Related projects

4.4.1. Xarray

As discussed in the introduction, xarray has inspired scipp heavily. After several rounds of prototyping the similarities had become so big that we chose to adopt the same terminology, such as Dataset and DataArray, to avoid cognitive overhead. We should thus justify the choice of not using xarray or not contributing changes to xarray. There is a number of aspects to consider:

(a) Physical units and propagation of uncertainties could be implemented with xarray using NEP-18\(^{15}\). This enhancement proposal for NumPy has been actively pushed by the xarray developers for these and similar purposes. In the case of propagating uncertainties this comes with a potentially big caveat: Apart from simple functions like addition and subtraction, equations for uncertainty propagation of, e.g., multiplication, are non-trivial and can result in a 10x or more loss of performance when implemented naively based on NumPy array arithmetics, due to the need for allocating temporary arrays and streaming through data multiple times. That is, for decent performance more work is required — to our understanding either (i) an essentially complete implementation of operations on arrays of data with uncertainties, i.e., exactly what we have done in scipp, or (ii) an implementation of a new dtype in NumPy, storing data as arrays of value/variance pairs.\(^{10}\)

(b) The type of sparse data required for handling event data is conceptually very different from dense NumPy arrays. Event data plays an absolutely central role for our current main objective, data reduction for neutron-scattering experiments. We do not just require support for event data but also high performance. Therefore we consider it essential that this component is written in C++ as opposed to Python.\(^{11}\) Since operations mixing dense and event data are also required, implementing an event data array on its own is not sufficient, since this would

\(^{9}\)an implementation of the “split-apply-combine” approach known from pandas and xarray, see [https://scipp.github.io/user-guide/groupby.html](https://scipp.github.io/user-guide/groupby.html).

\(^{10}\)Option (a) hints at a potential opportunity to leverage features of scipp with xarray. The __array_function__ from NEP-18 could be implemented for scipp’s Variable, bringing support for physical units and uncertainties when used in conjunction with xarray.

\(^{11}\)Event data as, e.g., an array of small NumPy arrays would not be adequate.
lack (fast) operations with NumPy arrays which are used for the dense data in xarray. That is, both have to be implemented, which already makes up a major part of code in scipp.

(c) Histograms and more specifically bin edges require storing coordinates in a data array or dataset that exceed the data extent by 1. This is not supported directly in xarray. There are certainly other options to do this, such as storing left and right bin edges as two coordinates or as a single coordinate storing a pair of the two, but this comes with other drawbacks and additional implementation effort. Bin-edge axes also allow for multi-dimensional histogramming, which will be part of a future version of scipp.

Essentially we consider the list of additional requirements on top of what xarray provides as too long and, in the case of event data as too fundamental. Effecting and contributing such fundamental changes to an existing framework is a long process and likely not obtained within the available time frame.

Furthermore, some of the requirements are unlikely to be obtainable within xarray itself since they may be incompatible with the project’s goals or philosophy.

4.4.2. Xtensor

The C++ library xtensor [16] provides data structures and operations similar to those in NumPy. Its key feature is the use of expression templates which allow for generation of efficient code for compound operations by, e.g., making good use of CPU caches and avoiding allocation of temporaries. It could thus be considered as a candidate to replace the lower-level components of scipp. However, since scipp relies on type-erasure to implement its higher-level concepts this is not possible in a convenient way — we are not aware of a way to combine expression templates and type erasure. A hypothetical use of xarray in scipp would thus have a small scope and would provide limited advantage. The transform mechanism with arbitrary lambdas described in Sec. 3.3.2 provides similar benefits to expression templates and is successfully combined with type erasure.

4.4.3. TensorFlow

While conceptually serving a different purpose, we mention TensorFlow [17] as a related project. TensorFlow supports dense, sparse, and ragged tensors. Scipp provides no equivalent to TensorFlow’s sparse tensors. The TensorFlow RaggedTensor is equivalent to nested variable-length lists, corresponding to scipp’s event data.

4.4.4. Mantid

As discussed throughout this article, scipp is to a large extent based on similar requirements as Mantid. Mantid is the current de facto standard for data reduction at many neutron scattering facilities. Mantid supports event data as well as dense data. It is highly specialized and dedicated for handling neutron (and muon) data. Multi-dimensional data is handled using MDHistoWorkspace and MDEventWorkspace but the support is less complete than for Mantid’s central data container, MatrixWorkspace, which provides a common interface for a list of histograms or a list of event lists. Workspaces provide uncertainty propagation for data values. Physical units are available only for the time-of-flight-derived axes. Data types and workspace contents are typically fixed and, e.g., multiple axes per dimension are not supported. Mantid’s TableWorkspace can hold any number of columns and is thus similar to a 1-D scipp dataset, but lacks support for coordinates and is not readily interoperable with other workspace types due a very different interface. Finally, WorkspaceGroup can be seen as an equivalent to scipp’s Dataset and allows for applying operations to multiple workspaces at once. It is actually even more generic since unlike Dataset it does not enforce coordinate alignment.

The functionality Mantid supports significantly exceeds scipp’s current capabilities. Functionality is accessible in C++ and via Python bindings. Most higher-level are encapsulated in so-called algorithms. A long history with explicit, detailed, and inflexible data structures has led to inconsistent, incomplete, and hard to use (Python) interfaces, as well as an inflation of the number of algorithms, making maintenance increasingly harder. Several years of work on data handling for ESS — a new facility which needs to commission more than ten new instruments over the coming years [18] — has proven that necessary changes to Mantid are often time-consuming or out-right impossible. Furthermore, long training times and the recurrent need to make deep changes in Mantid due to lacking features or data access in the Python interfaces made it increasingly risky to continue relying solely on

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12before ESS operations start, i.e., a couple of years
Mantid during the ESS hot-commissioning phase. On the plus side, when used via the graphical user interfaces for existing and well-supported instruments at existing facilities, Mantid is very powerful and full-featured. As the de facto standard, Mantid encapsulates more than a decade’s worth of knowledge about handling neutron-scattering data. The scipp project aims to leverage this by using Mantid as a Python library for specialized tasks. Current examples of this are loading NeXus files and sample-geometry-based corrections such as absorption corrections. scipp’s goal is not to fully replace Mantid—we rather foresee that the two projects will continue to live in parallel, exploiting synergies and, for some aspects, living in symbiosis.

5. Conclusion and outlook

We have presented an early version of the scipp library. scipp provides comparatively simple data structures alongside a set of generic operations. With flexibility designed into the data structures, it can nevertheless be a powerful tool to tackle many tasks involving scientific data. For example, scipp appears to be capable of adequately representing and processing neutron-scattering data without the need for dedicated data structures, and with reduced need for dedicated algorithms. A number of scipp’s features discussed throughout this article already surpasses the current scope of Mantid. What is lacking is, e.g., support for the multitude of specialized correction algorithms that Mantid provides, but users of scipp can rely on manual or automatic conversion of data from Mantid to scipp. For example, we reuse Mantid algorithms that rely on advanced geometry operations by providing wrappers which setup the input workspaces and convert output workspaces back to scipp.

While scipp is and will be kept generic, development effort is currently focussed on concrete feature and performance requirements for data reduction at the ESS. That is, while we are consolidating common basics, significant amounts of work will be going into event-data handling and performance improvements in operations with event data. To avoid going off on a tangent, we are using real workflows — initially data reduction for an ESS powder diffractometer with several million pixels and event rates exceeding $10^7$ neutrons/s — to steer and drive development. As discussed in Sec. 4.1, a naive implementation typically ends up being bandwidth-bound. When reaching that point we will evaluate the balance between I/O and computation for the aforementioned model workflow. This will flow into a decision on which parallelization strategies to focus on. Other future work will include direct support for loading and saving files as well as an improved interface for working with event data or other unaligned data.

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References

[1] S. Heybrock, O. Arnold, I. Gudich, D. Nixon and N. Vaytet, Scipp Documentation, 2020. https://scipp.github.io/.
[2] S. Heybrock, O. Arnold, I. Gudich, D. Nixon and N. Vaytet, Scipp GitHub, 2020. https://github.com/scipp/scipp.
[3] W. McKinney, Data Structures for Statistical Computing in Python, in: Proceedings of the 9th Python in Science Conference, S. van der Walt and J. Millman, eds, 2010, pp. 51–56.
[4] S. Hoyer and J. Hamman, xarray: N-D labeled arrays and datasets in Python, Journal of Open Research Software 5(1) (2017). doi:10.5334/jors.148.
[5] T. Kluyver, B. Ragan-Kelley, F. Pérez, B. Granger, M. Bussonnier, J. Frederic, K. Kelley, J. Hamrick, J. Grout, S. Corlay, P. Ivanov, D. Avila, S. Abdalla and C. Willing, Jupyter Notebooks – a publishing format for reproducible computational workflows, in: Positioning and Power in Academic Publishing: Players, Agents and Agendas, F. Loizides and B. Schmidt, eds, IOS Press, 2016, pp. 87–90.
[6] O. Arnold, J.C. Bilheux, J.M. Borreguero, A. Buts, S.I. Campbell, L. Chapon, M. Doucet, N. Draper, R.F. Leal, M.A. Gigg, V.E. Lynch, A. Markvardsen, D.J. Mikkelson, R.L. Mikkelson, R. Miller, K. Palmen, P. Parker, G. Passos, T.G. Perring, P.F. Peterson, S. Ren, M.A. Reuter, A.T. Savici, J.W. Taylor, R.J. Taylor, R. Tolchenov, W. Zhou and J. Zikovsky, Mantid — Data analysis and visualization package for neutron scattering and μSR experiments, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 764 (2014), 156–166. doi:https://doi.org/10.1016/j.nima.2014.07.029.
[7] P.F. Peterson, S.I. Campbell, M.A. Reuter, R.J. Taylor and J. Zikovsky, Event-based processing of neutron scattering data, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 803 (2015), 24–28. doi:https://doi.org/10.1016/j.nima.2015.09.016.
[8] J. Wenzel, R. Jason and M. Dean, pybind11 – Seamless operability between C++11 and Python, 2017, https://github.com/pybind/pybind11.

[9] J.D. Hunter, Matplotlib: A 2D graphics environment, Computing in Science & Engineering 9(3) (2007), 90–95. doi:10.1109/MCSE.2007.55.

[10] M. Könnecke, F.A. Akeroyd, H.J. Bernstein, A.S. Brewster, S.I. Campbell, B. Clausen, S. Cottrell, J.U. Hoffmann, P.R. Jemian, D. Männicke, R. Osborn, P.F. Peterson, T. Richter, J. Suzuki, B. Watts, E. Wintersberger and J. Wuttke, The NeXus data format, Journal of Applied Crystallography 48(1) (2015), 301–305. doi:10.1100/1600576714027575.

[11] A. O’Dwyer, What is Type Erasure? 2020. https://quuxplusone.github.io/blog/2019/03/18/what-is-type-erasure/.

[12] P. Perkelbauer, S. Parent, M. Marcus and B. Stroustrup, Runtime Concepts for the C++ Standard Template Library, in: Proceedings of the 2008 ACM Symposium on Applied Computing, SAC ’08, ACM, New York, NY, USA, 2008, pp. 171–177. ISBN 978-1-59593-753-7. doi:10.1145/1363686.1363734.

[13] Dask Development Team, Dask: Library for dynamic task scheduling, 2016. https://dask.org.

[14] B. Schling, The Boost C++ Libraries, XML Press, 2011. ISBN 0982219199, 9780982219195.

[15] S. Hoyer, M. Rocklin, M. van Kerkwijk, H. Abbase and E. Wieser, NEP 18 — A dispatch mechanism for NumPy’s high level array functions, 2018, https://numpy.org/neps/nep-0018-array-function-protocol.html.

[16] QuantStack, xtensor — The C++ Tensor Algebra Library, 2019. https://xtensor.readthedocs.io.

[17] M. Abadi, A. Agarwal, P. Barham, E. Brevdo, Z. Chen, C. Citro, G.S. Corrado, A. Davis, J. Dean, M. Devin, S. Ghemawat, I. Goodfellow, A. Harp, G. Irving, M. Isard, Y. Jia, R. Jozefowicz, L. Kaiser, M. Kudlur, J. Levenberg, D. Mané, R. Monga, S. Moore, D. Murray, C. Olah, M. Schuster, J. Shlens, B. Steiner, I. Sutskever, K. Talwar, P. Tucker, V. Vanhoucke, V. Vasudevan, F. Viégas, O. Vinyals, P. Warden, M. Wattenberg, M. Wicke, Y. Yu and X. Zheng, TensorFlow: Large-Scale Machine Learning on Heterogeneous Systems, 2015, Software available from tensorflow.org. http://tensorflow.org/.

[18] K.H. Andersen, D.N. Argyriou, A.J. Jackson, J. Houston, P.F. Henry, P.P. Deen, R. Toft-Petersen, P. Beran, M. Strobl, T. Arnold, H. Wacklin-Knecht, N. Tsapatsaris, E. Oksanen, R. Worsacek, W. Schweika, D. Mannix, A. Hiess, S. Kennedy, O. Kirstein, S.P. Årsköld, J. Taylor, M.E. Hagen, G. Laszlo, K. Kanaki, F. Piscitelli, A. Khaplanov, I. Stefanescu, T. Kittelmann, D. Pfeiffer, R. Hall-Wilton, C.I. Lopez, G. Aprigliano, L. Whitelegg, F.Y. Moreira, M. Olsson, H.N. Bordallo, D. Martin-Rodriguez, H. Schneider, M. Sharp, M. Hartl, G. Nagy, S. Ansell, S. Pullen, A. Vickery, A. Fedrigio, F. Mezei, M. Arai, R.K. Heenan, W. Halcrow, D. Turner, D. Raspino, A. Orszulik, J. Cooper, N. Webb, P. Galsworthy, J. Nightingale, S. Langridge, J. Elmer, F. Frielingshaus, R. Hanslik, A. Gussen, S. Jaksch, R. Engels, T. Kozielewski, S. Butterweck, P. Feygenson, P. Harbott, A. Poqué, A. Schweab, K. Lieutenant, N. Violini, J. Voigt, T. Brückel, M. Koenen, H. Kämmerling, E. Babcock, Z. Salhi, A. Wischniewski, A. Heynen, S. Désert, J. Jestin, F. Porcher, X. Fabrèges, G. Fabrèges, B. Annighöfer, S. Klimko, T. Dupont, T. Robillard, A. Goukassov, S. Longeville, C. Alba-Simionesco, P. Bourges, J.G.L. Bouffy, P. Lavie, S. Rodrigues, E. Calzada, M. Lerche, B. Schillinger, P. Schmakan, M. Schulz, M. Seifert, W. Lohstroh, W. Freti, J. Neuhaus, L. Loaiza, A. Tartaglione, A. Glicine, S. Schütz, J. Stahn, E. Lehmann, M. Morgan, J. Schefer, U. Figes, R. Lauter, C. Niedermayer, F. Fenske, G. Nowak, M. Rouijaa, D.J. Siemens, R. Kiehn, M. Müller, H. Carlsten, L. Udy, K. Lefmann, J.O. Birk, S. Holm-Dahlin, M. Bertelsen, U.B. Hansen, M.A. Olsen, M. Christensen, K. Iversen, N.B. Christensen, H.M. Rønnow, P.F. Freeman, B.C. Hauback, R. Kollevatov, I. Llamas-Jansa, A. Orecchi, F. Sacchetti, A. Petillo, A. Paciaroni, P. Tozzi, M. Zanatta, P. Luna, I. Herranz, O.G. del Moral, M. Huerta, M. Magán, M. Mosconi, E. Abad, J. Aguilar, S. Stepanyan, G. Bakedano, R. Vivanco, I. Bustinduy, F. Sordo, J.L. Martínez, R.E. Lechner, F.J. Villacorta, J. Saroun, P. Lukiš, M. Markó, M. Zanetti, S. Bellissima, L. del Rosso, F. Mas, C. Bovo, M. Choudhary, A.D. Bonis, L.D. Fresco, C. Scatigno, S.F. Parker, F. Fernandez-Alonso, D. Colognesi, R. Senesi, C. Andreani, G. Gori, G. Sciotti and A. Schreyer, The instrument suite of the European Spallation Source, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 957 (2020), 163402. doi:https://doi.org/10.1016/j.nima.2020.163402. http://www.sciencedirect.com/science/article/pii/S0168900220300897.