EUROPEAN
SPALLATION
SOURCE

Scipp

Scientific C++ and Python libraries for labeled multi-dimensional data

Simon Heybrock

simon.heybrock@esss.se

Contributors:

Owen Arnold Igor Gudich Daniel Nixon Neil Vaytet

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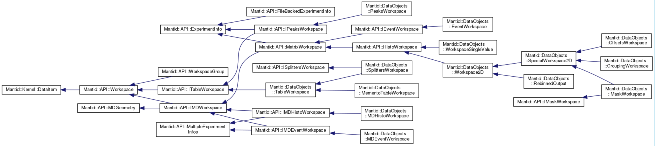
Mantid Workspace hierarchy: restrictive, large, and complicated



Wish list

- Easy to learn and *remember*, obvious interfaces.
  - Usable by anyone who knows some Python.
  - But also not getting in the way or overly restrictive for experts.
- Flexible and accessible data structures.
  - Data and metadata content available at a glance.
  - Quick to inspect and visualize data.
  - Can store anything.
- Fast prototyping, give scientists tools to experiment with their data.

Requirements

Must-have features

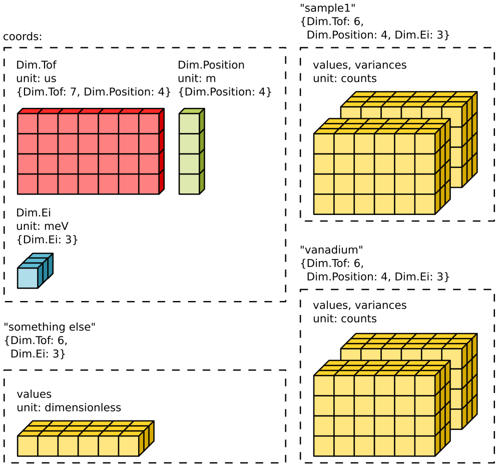
Carried over and evolved from Mantid:

1. Physical units *everywhere*.
2. Propagation of uncertainties.
3. Support for histograms, in particular bin-edges.
4. Event-data, a special case of sparse data (raw data later converted to histograms[1]).
5. `C++` backend for interfacing with existing `C++` codebases, performance opportunities.

[1] random-length list of events at each coordinate point, each event described by typically 1-4 small fields, e.g., `double`

Self-describing data using scipp

scipp's[2] Dataset, inspired by xarray (xarray.pydata.org):



[2] Etymology: Scientific C++ library → Sci++ → scipp

Anatomy of operations with scipp.Dataset

```
delta = d['a']                                  d['b']

             (1)                                  (1)
```

Natural and implicit:

1. Select dataset entries by name.

Anatomy of operations with scipp.Dataset

```
delta = d['a'][Dim.Pixel, 7:42]          d['b']

              (1)          (2)                        (1)
```

Natural and implicit:

1. Select dataset entries by name.
2. Slice based on named dimension.

Anatomy of operations with scipp.Dataset

```
delta = d['a'][Dim.Pixel, 7:42]   mean(d['b'], Dim.Energy)

            (1)          (2)          (4,5)  (1)     (3)
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Natural and implicit:

1. Select dataset entries by name.
2. Slice based on named dimension.
3. Named dimensions for other ops, e.g., mean over given dim.

Anatomy of operations with scipp.Dataset

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5. Handling of physical units.

Anatomy of operations with scipp.Dataset

```
delta = d['a'][Dim.Pixel, 7:42] - mean(d['b'], Dim.Energy)

              (1)         (2)      (4-8)(4,5)  (1)      (3)
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Natural and implicit:

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3. Named dimensions for other ops, e.g., mean over given dim.
4. Propagation of uncertainties.
5. Handling of physical units.
6. Matching of coordinates.

Anatomy of operations with scipp.Dataset

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7. Broadcasting into missing dimensions.

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8. Transposing matching dimensions.

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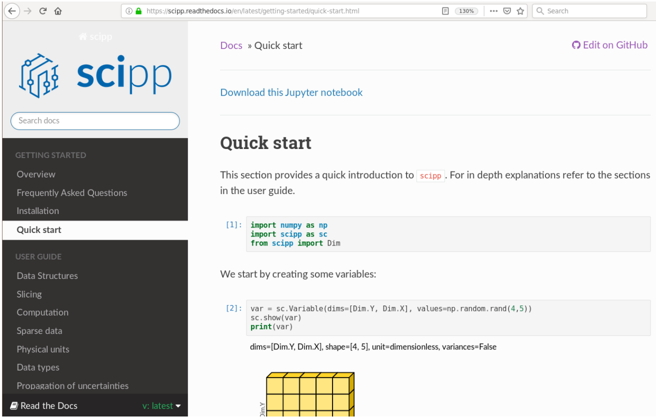
8. Transposing matching dimensions.

⇒ Free up mental capacity for the important things (science).

Example: Quick start (Jupyter notebook)

https://scipp.readthedocs.io/en/latest/getting-started/quick-start.html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scipp

Search docs

GETTING STARTED
Overview
Frequently Asked Questions
Installation
Quick start

USER GUIDE
Data Structures
Slicing
Computation
Sparse data
Physical units
Data types
Propagation of uncertainties

Read the Docs v: latest

Docs » Quick start

Edit on GitHub

Download this Jupyter notebook

Quick start

This section provides a quick introduction to `scipp`. For in depth explanations refer to the sections in the user guide.

[1]:
```
import numpy as np
import scipp as sc
from scipp import Dim
```

We start by creating some variables:

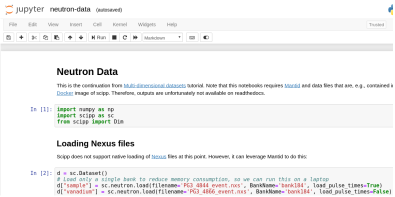
[2]:
```
var = sc.Variable(dims=[Dim.Y, Dim.X], values=np.random.rand(4,5))
sc.show(var)
print(var)
```

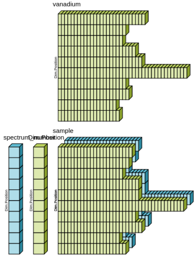
dims=[Dim.Y, Dim.X], shape=[4, 5], unit=dimensionless, variances=False

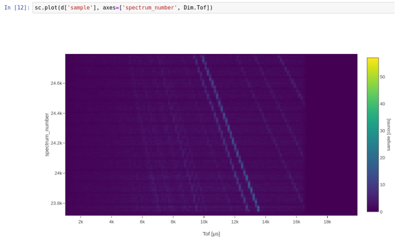
Dim.Y

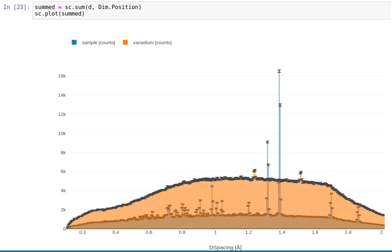
Example: Sparse data and neutrons (Jupyter notebook)

https://github.com/scipp/scipp-neutron-jupyter-demo
https://mybinder.org/v2/gh/scipp/scipp-neutron-jupyter-demo/master









About scipp

`scipp-units`	Physical units library, based on `boost-units`.
`scipp-core`	Core library with basic and generic operations.
`scipp-neutron`	Neutron-scattering specifics based on `scipp-core`, e.g., unit conversions.

. . . and more in the future?

Fact sheet

- C++17, Python bindings with pybind11
- 10 kLOC (`C++`) and 4 kLOC (`Python`)
  - not counting tests and documentation
- Jupyter notebooks with various visualization options
- Install using conda or docker
- Single threaded and not optimized at this point

Status and plan

- 2018: design and prototyping.
- First demo to wider audience in April 2019.
- Major refactor and cleanup of public interface and internals.
  - Conceptual changes → closer to `xarray` API.
- 0.1 release last month. This release is *intended for experimental use* and has *many limitations*.

Next

Continue work on core libraries, focus more on sparse data and performance.

- Using a *real workflow* to *drive and steer* development...
- ...thus avoid going off on a tangent.
- Determine what (if any) kind of parallelization beyond multi-threading required for our application. `dask`?

Conclusion

Summary

- scipp aimed at providing better and less error-prone processing of scientific data.
- Still a long way to go, but chiming in early could ensure that this does not become a specialized solution.
  ⇒ Comments and questions welcome!

Documentation:

- https://scipp.readthedocs.io
  - Download documentation pages as Jupyter notebooks.

Project home:

- https://github.com/scipp/scipp
  - Run scipp using Binder → notebook without installation.

Backup slide 1: Why not contribute to `xarray`?

Why not contribute to `xarray`?

- Too many additional requirements.
- Therefore not realistically achievable within the time frame(?).
- Some of the requirements are unlikely to be obtainable within `xarray`.

⇒ Focus on *interoperability* instead of reuse

- Good `NumPy` compatibility.
- May wrap `scipp.Dataset` ⇒ can use subset of `xarray.Dataset` functionality.
  - Successful proof of concept using `xarray` plotting.
  - Possible if a dataset does not use features beyond `xarray`'s.
- Potential for collaboration on subsets of functionality.