Object-Oriented Data Analysis Environment for Neutron Scattering

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(**J**apan **P**roton **A**cceleration **R**esearch **C**omplex / **M**aterials and **L**ife Science **F**acility)

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for Neutron Scattering.

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1, J-PARC / MLF

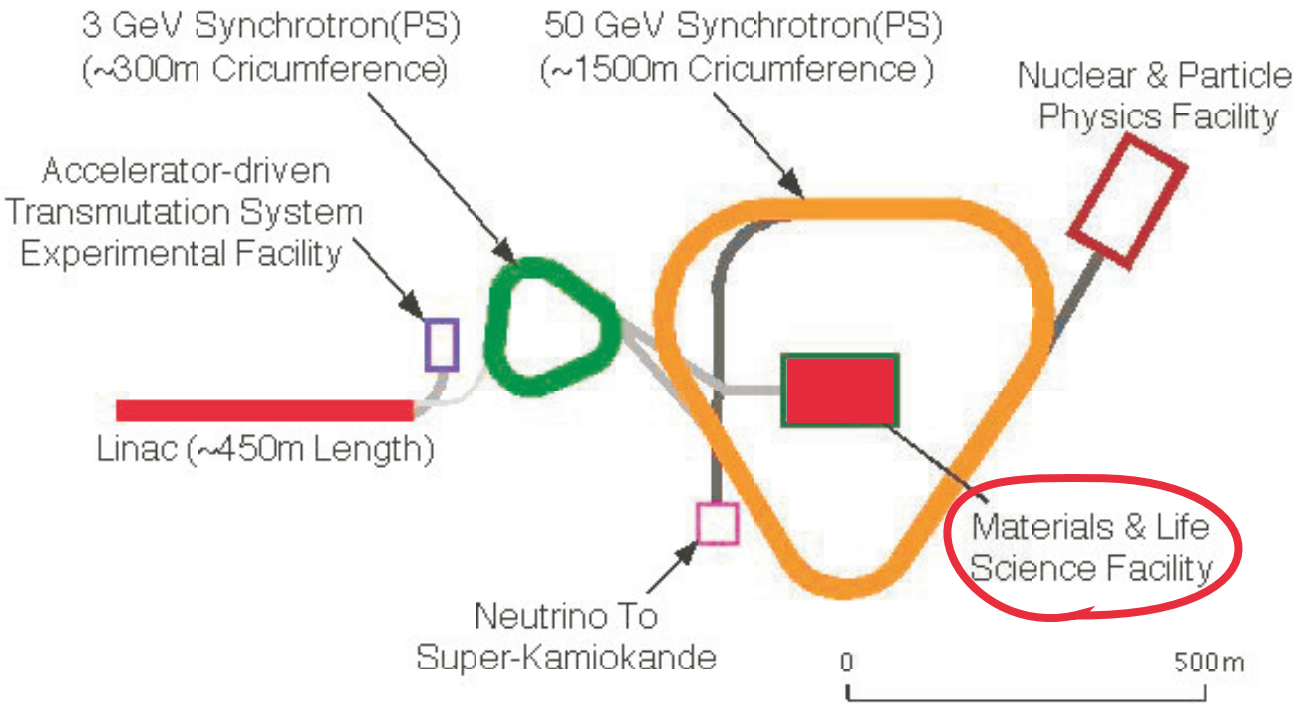
Current Facility of Pulsed Neutron Scattering --- KENS of KEK
have been operated since 1980.
is the first facility in the world.

Its operating neutron beam power is 3kW.
ISIS (Rutherford Appleton Lab. UK) 160kW.

J-PARC / MLF

is constructing at Tokai campus of JAERI (Japan Atomic Energy Research Institute) by KEK and JAERI.

The operation for user will be started on 2007.
Its beam power will be 1MW.
--- the highest intensity beam power in the world



High Intensity Proton Accelerator Project

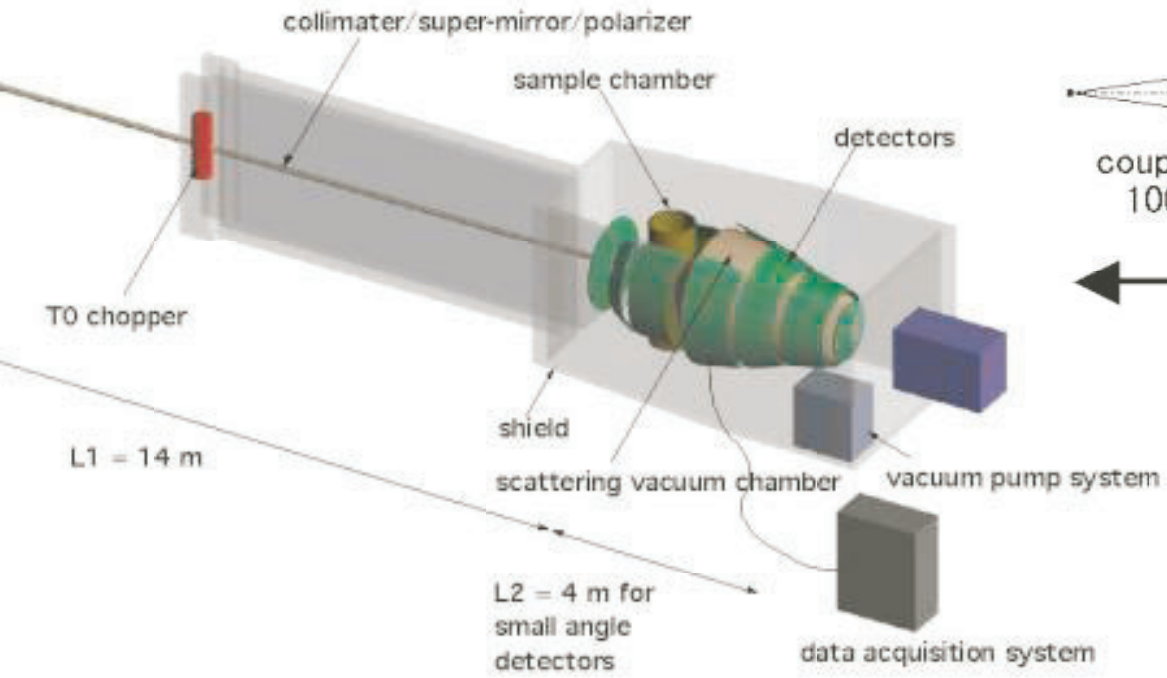
High Intensity Proton Accelerator Facility, J-PARC, aims to pursue frontier science in particle physics, materials and life-science and nuclear technology, using a new proton accelerator complex.

The Material and Life Science Facility, MLF, is a user facility providing a neutron source for experiments of materials and life sciences.

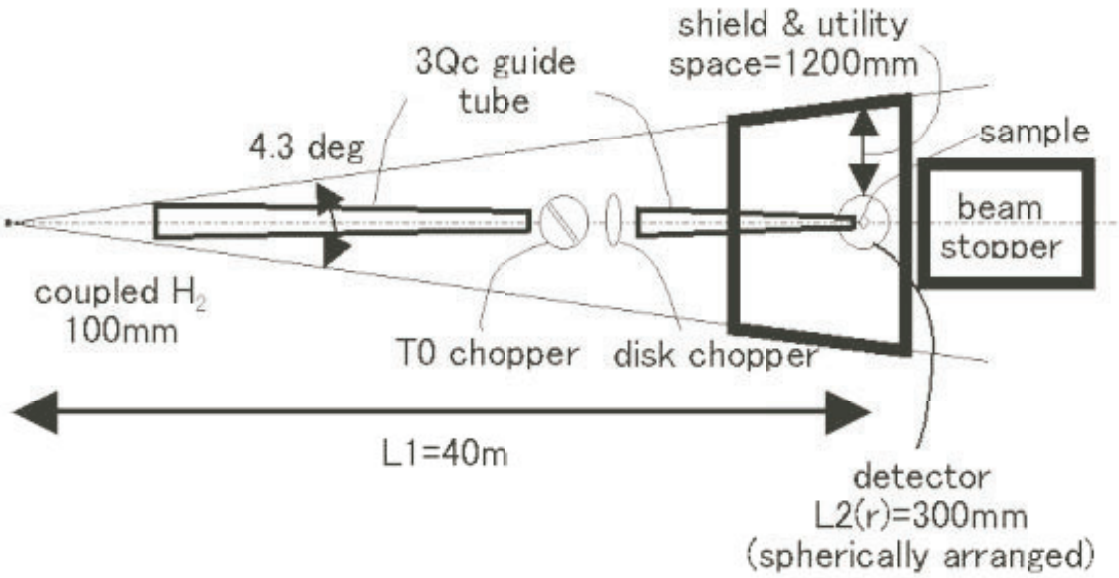
Twenty-three instruments,
Many types of instruments will be installed in MLF.

All experimental components have to be applied to each instrument.

Hardware control, Data analysis tools, Simulation tools, ...



Total scattering diffractometer



Single crystal diffractometer
for biological materials

The estimation of the user and instrument activity in MLF.

The number of users

100 users / day 200 days / year

The time period of each experiment.

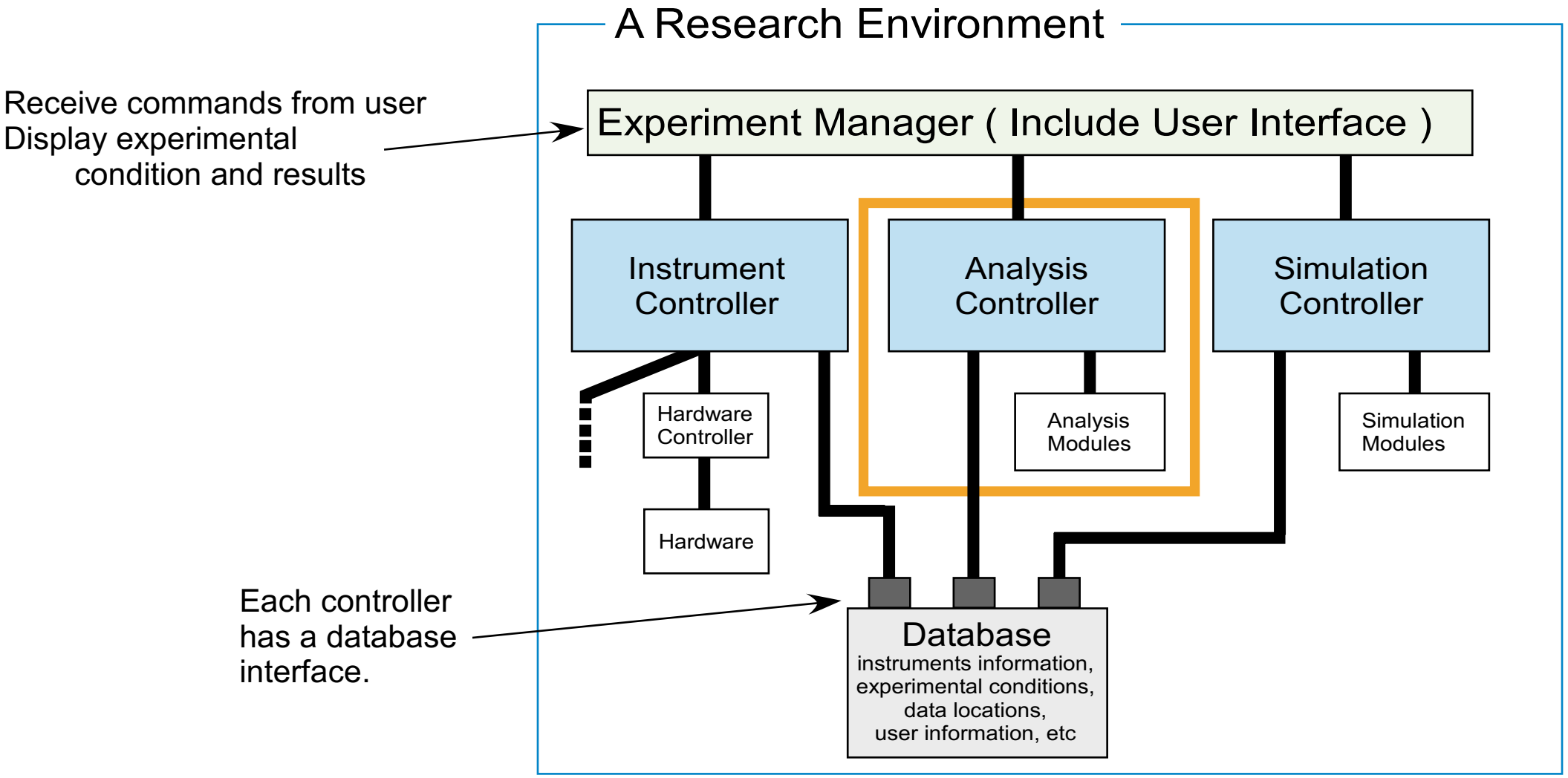
---- include the time of setup.

0.5 - 2 days / group

The established total experimental environment must be provided by the facility side.

2, Computer-assisted Research Environment for Neutron Scattering.

The research environment should be
a framework, which unifies all experimental components.



3, Design of Analysis Package

Current Way of Analysis

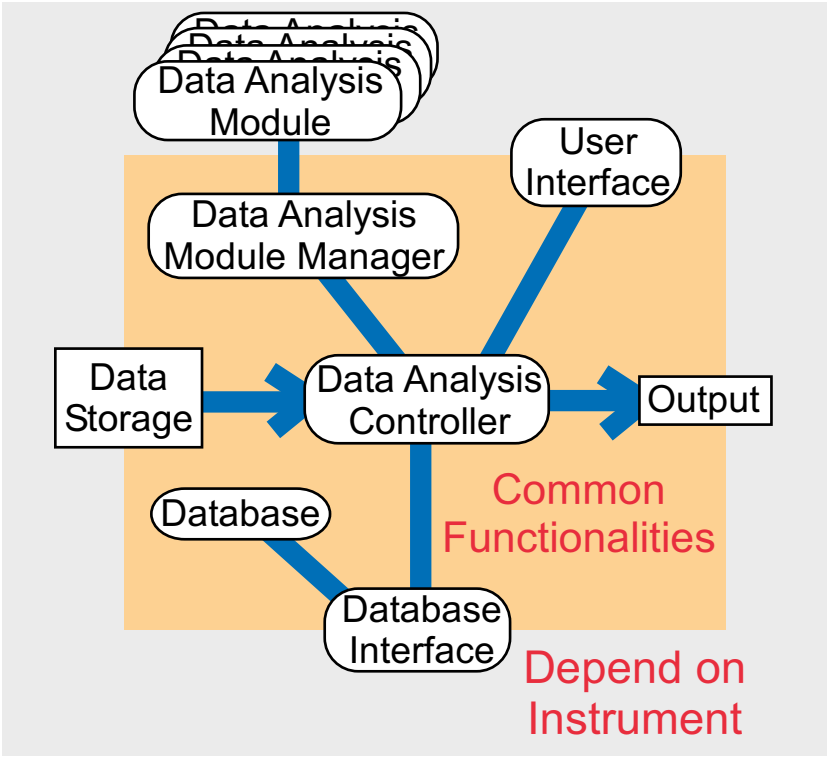
* Number of analysis softwares specific to instruments have been developed.
  -- It is far from making good use of software resources.

Our New Concept of Data Analysis Environment

* We provide a framework, which has
  common and generic analysis functionalities .

* We take full advantage of
  Object-Oriented methodology in;
  - Object-Oriented Analysis / Design
  - Rapid prototyping, spiral approach.

* Various merits of Object-Oriented approach help us.
  - requirements of **keeping good software for a long time**
  - safe access to data
  - obvious definition of common functionalities



The Aim of this Framework

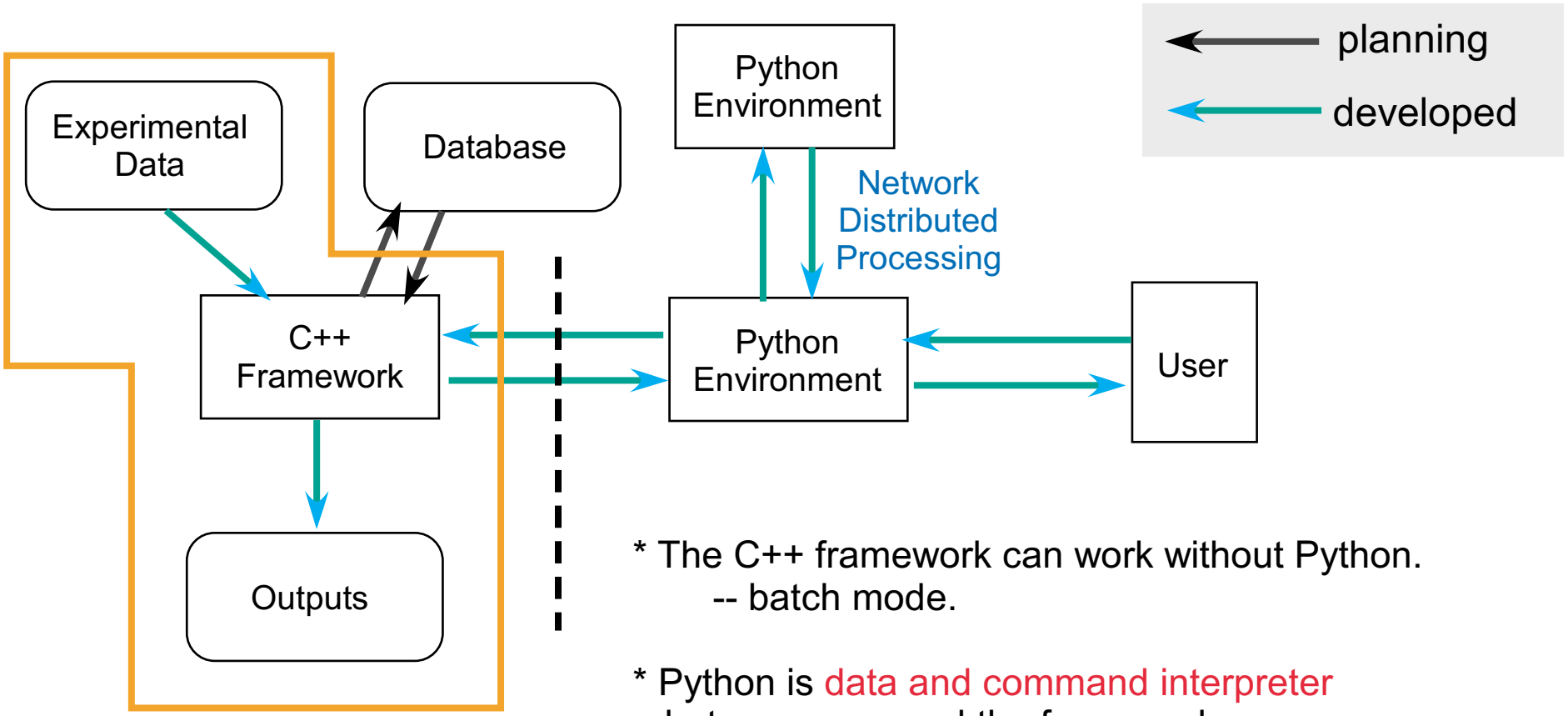
Standard framework for analysis software in MLF (and another facilities).
-- required good-performance in on- and off-line data analysis.
---> batch mode, interactive mode
-- confirm to run on various systems.

Prepare network distributed processing environment.

Required to handle large scale data in high performance.
-- provide efficient and good-scalable data container.

Satisfy these requirements ---- C++
Python

The Structure of Analysis Package

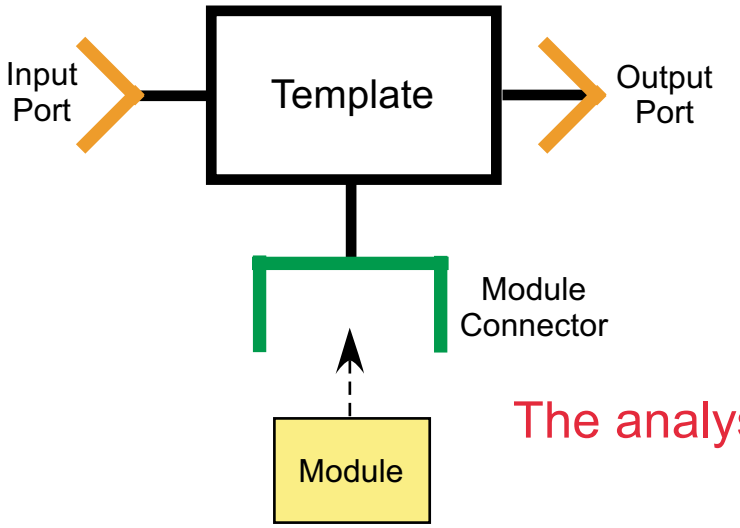


* The C++ framework can work without Python.
  -- batch mode.

* Python is data and command interpreter between user and the framework.
  -- interactive mode.

* Network distributed processing environment is provided with Python.

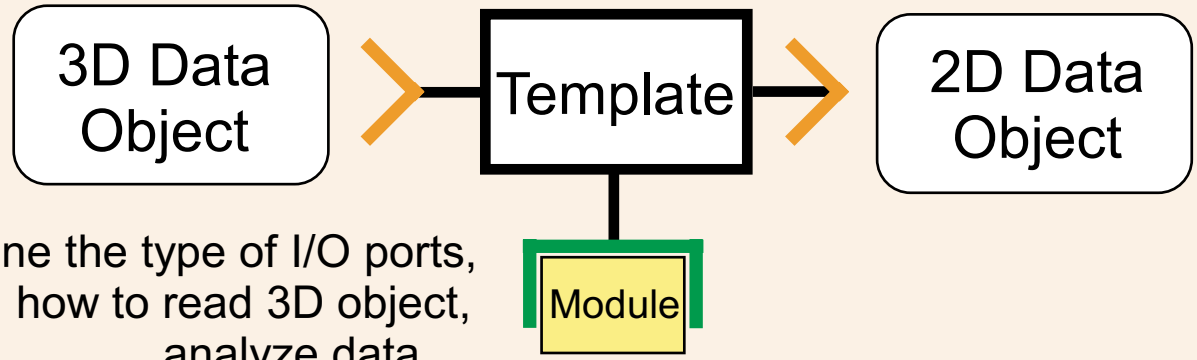
The Design Concept of Analysis Function



The analysis function template has Input / Output-port and Module-Connector.

The analysis module is provided for each use case.

An example of use case -- reduction of data dimension



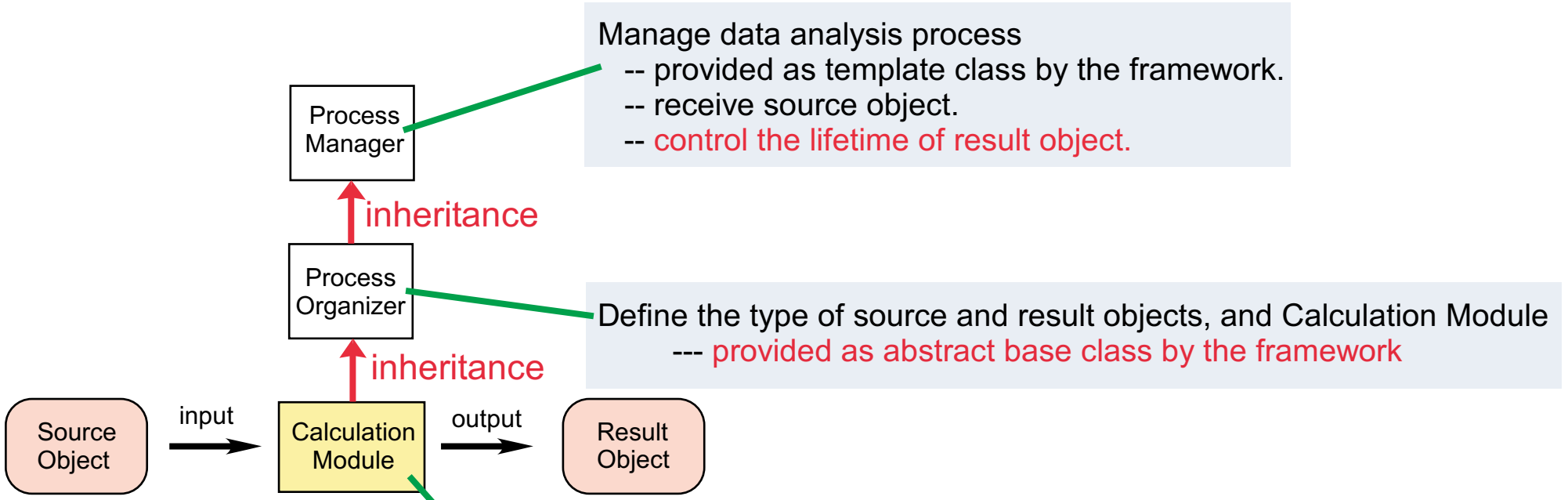
Define the type of I/O ports, how to read 3D object, analyze data, make 2D object

Paying less attention to data flow

Design of a set of analysis functions

A schematic example of the basic and simple use case

An analysis functionality is organized
by using relationship of multiple inheritance.



Manage data analysis process
-- provided as template class by the framework.
-- receive source object.
-- control the lifetime of result object.

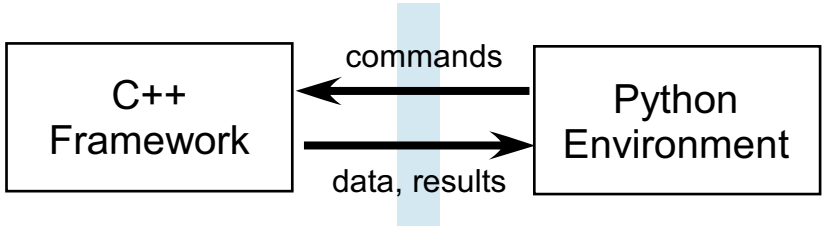
Define the type of source and result objects, and Calculation Module
--- provided as abstract base class by the framework

Define concrete method of each use case.

Generic and common functionality --- by the framework.
The functionality specific to instruments --- by the user side.

User Interface -- Python Environment

* The interface between C++ and Python is created by SWIG.
(Simplified Wrapper and Interface Generator --- http://www.swig.org/).



Interface created by SWIG

Why Python is selected as user interface ?

* Python is an object-oriented and interactive programing language.

---- Python is easily adapted for C++ framework.

---- Interactive user interface is useful
for developing application software on the framework.

* Many scientific and mathematical tools on Python have been developed.
ex. plotting library, mathematical library .....

* Analysis software in SNS is developing with C and Python,
we can cooperate in developing software.

SNS is an accelerator-based neutron source being built in Oak Ridge, US.

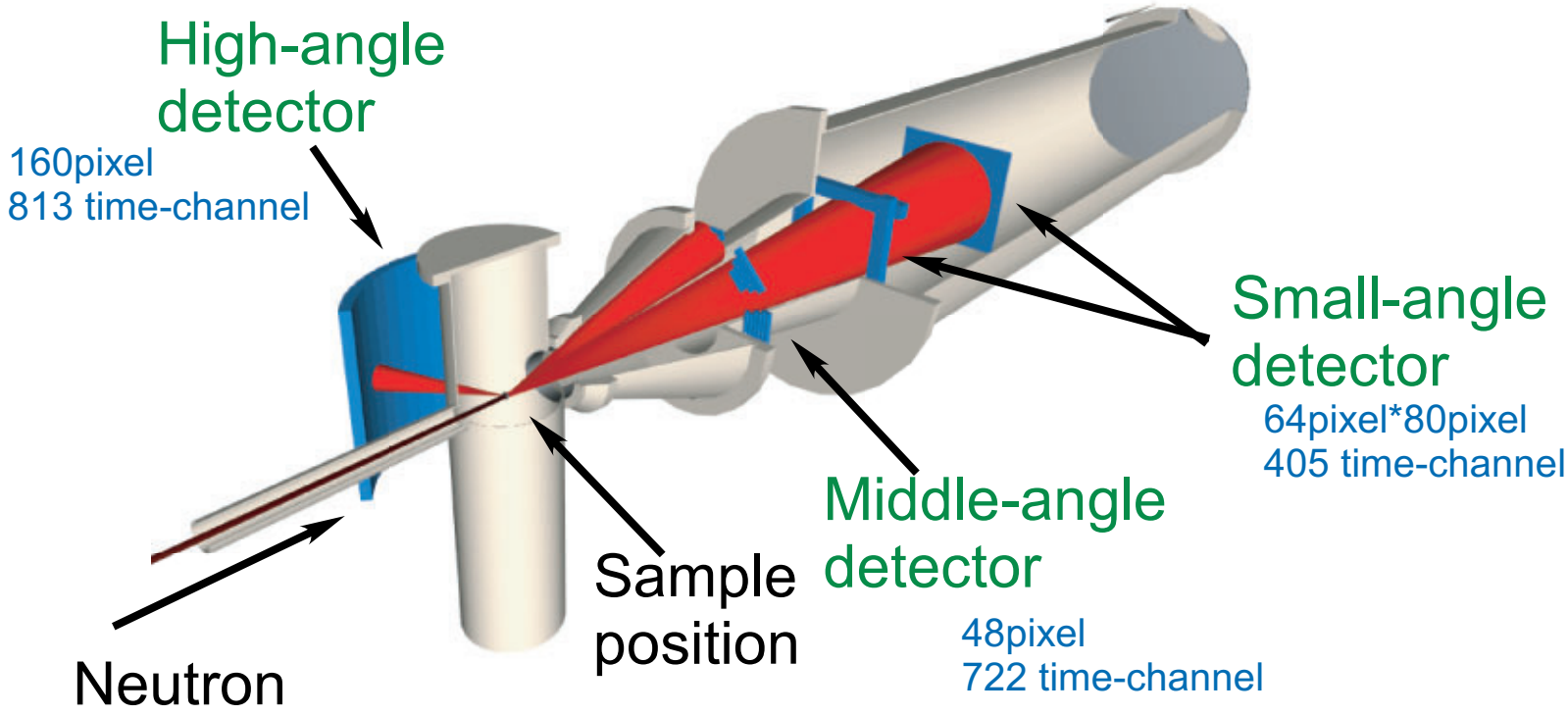
4, An Application to the SWAN Real Experiment .

Setting up data analysis software for SWAN on the framework.

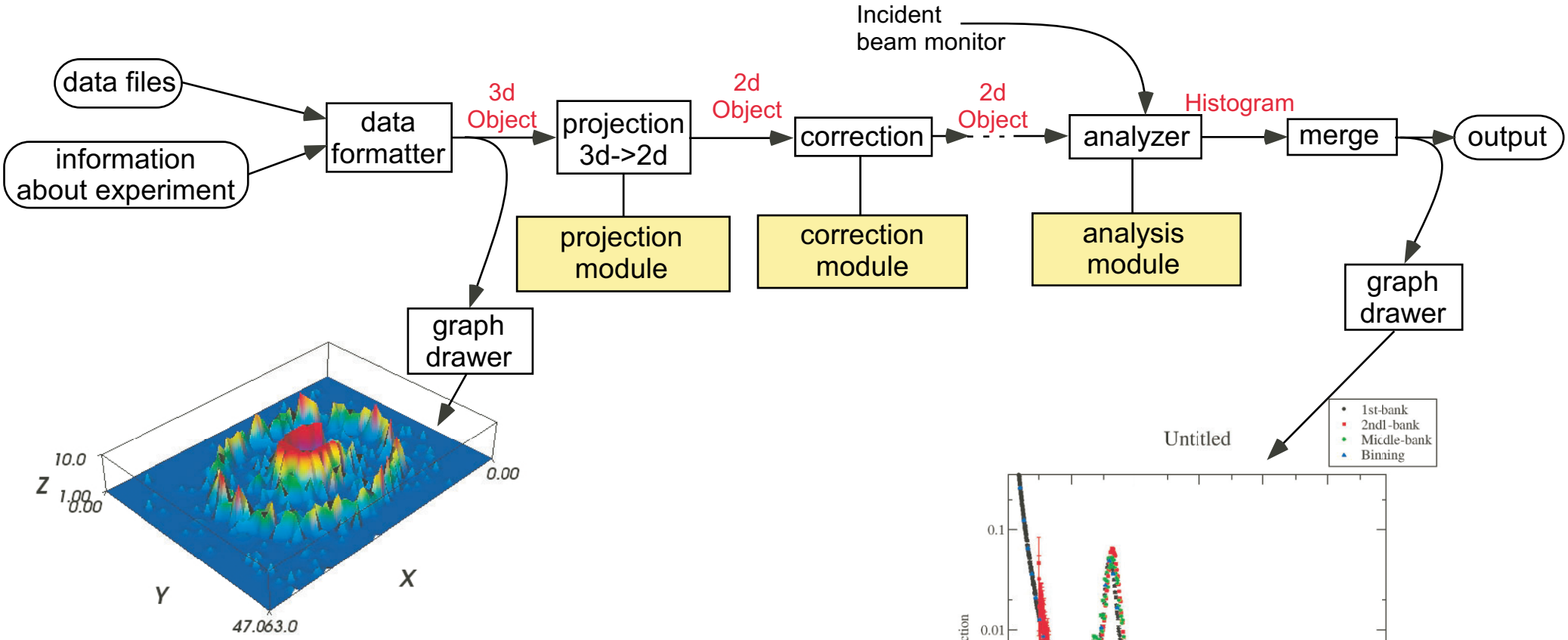
(SWAN : **S**mall/**W**ide **A**ngle **N**eutron Scattering Diffractmeter
at Neutron Scattering Facility of KEK)

* Each detector geometry requires to provide its proper analysis method.

* Three detector banks are installed
to obtain wide range (0.05 - 100nm) structural information.
(emulsion, biological - , magnetic-materials, ...)



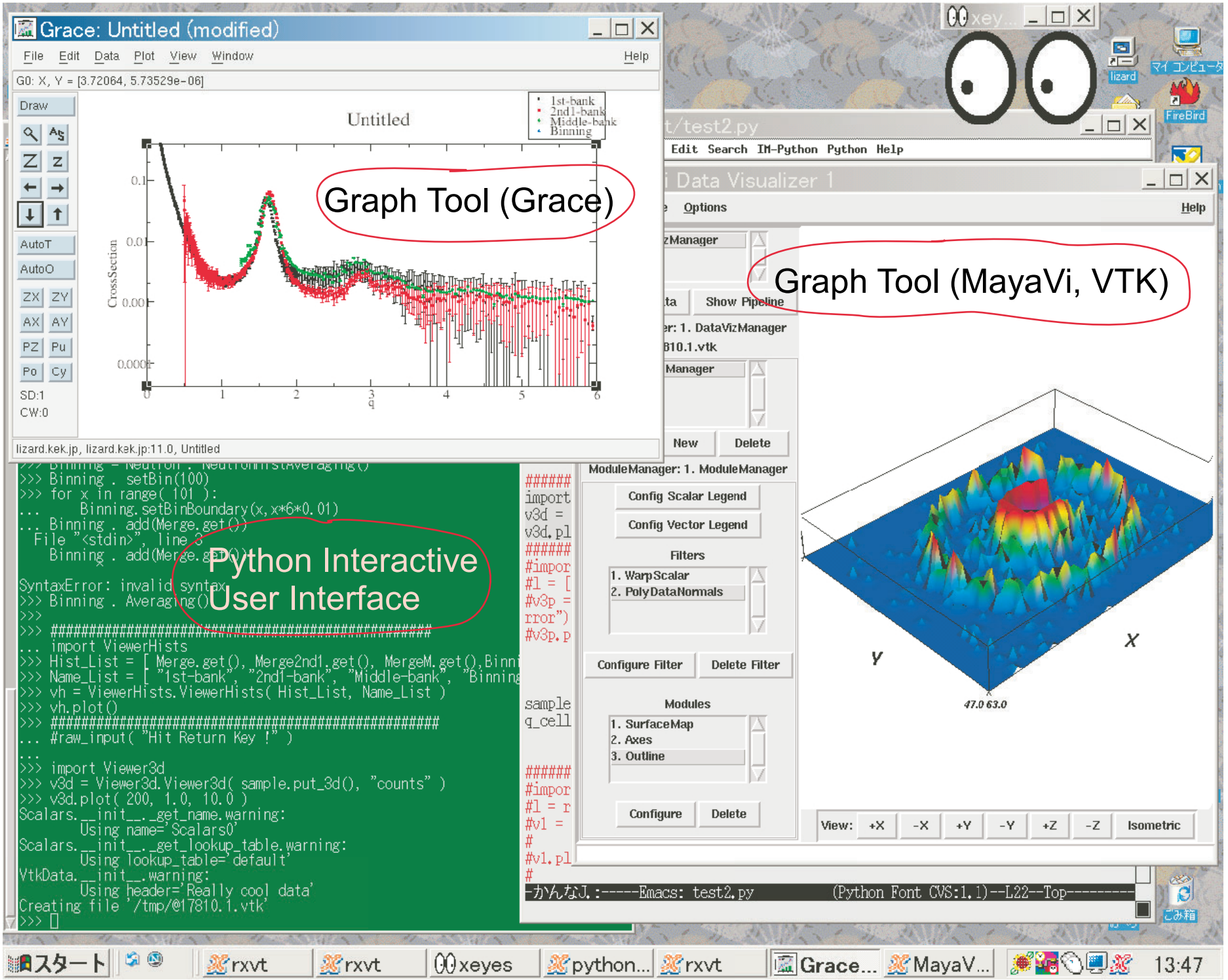
Analysis Flow Diagram for SWAN



The application is designed / executed on Python.

Each module is prepared to apply each functionality.

Data objects are common formats of the framework.


Grace: Untitled (modified)
File Edit Data Plot View Window Help
G0: X, Y = [3.72064, 5.73529e-06]
Draw
AutoT
AutoO
ZX ZY
AX AY
PZ Pu
Po Cy
SD:1
CW:0
Untitled
1st-bank
2nd1-bank
Middle-bank
Binning
CrossSection
q
lizard.kek.jp, lizard.kek.jp:11.0, Untitled
Graph Tool (Grace)
Python Interactive User Interface
>>> Binning . setBin(100)
>>> for x in range(101):
... Binning.setBinBoundary(x,x*6*0.01)
... Binning . add(Merge.get())
SyntaxError: invalid syntax
>>> Binning . Averaging()
>>> ##
... import ViewerHists
>>> Hist_List = [Merge.get(), Merge2nd1.get(), MergeM.get(),Binni
>>> Name_List = ["1st-bank", "2nd1-bank", "Middle-bank", "Binning
>>> vh = ViewerHists.ViewerHists(Hist_List, Name_List)
>>> vh.plot()
>>> ##
... #raw_input("Hit Return Key !")
>>> import Viewer3d
>>> v3d = Viewer3d.Viewer3d(sample.put_3d(), "counts")
>>> v3d.plot(200, 1.0, 10.0)
Scalars.__init__._get_name.warning:
Using name='Scalars0'
Scalars.__init__._get_lookup_table.warning:
Using lookup_table='default'
VtkData.__init__.warning:
Using header='Really cool data'
Creating file '/tmp/@17810.1.vtk'
>>>
Edit Search IM-Python Python Help
Data Visualizer 1
Options
Help
Show Pipeline
New
Delete
ModuleManager: 1. ModuleManager
Config Scalar Legend
Config Vector Legend
Filters
1. WarpScalar
2. PolyDataNormals
Configure Filter
Delete Filter
Modules
1. SurfaceMap
2. Axes
3. Outline
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Graph Tool (MayaVi, VTK)
Y
X
47.0 63.0
View: +X -X +Y -Y +Z -Z Isometric
-かんなJ.:-----Emacs: test2.py (Python Font CVS:1.1)--L22--Top---------
スタート
rxvt
rxvt
xeyes
python...
rxvt
Grace...
MayaV...
13:47

5, Summary.

1, We have developed an analysis framework
for neutron scattering experiments,
based on Object-Oriented approach.

2, The framework provides common and generic data analysis functionalities
for all neutron scattering instruments.

3, We applied the framework to the analysis of a real experiment.
The application is well working.

Under developing components are;
- graphical user interface
- database connection
- network distributed processing.

If you want to get further information about this project,
please see http://research.kek.jp/group/cred/

Analysis Package (C++) consists of 6 groups.

* System — Data container, Data Input / Output
* Calculation — Basic calculation tools

Setup the environment of analysis package,
provide basic tools.

* Correction — Correction of observed data
* Projection — Reduction of data dimensions
* Merge — Merging data sets
  Integration of data sets
* Analyzer — Extracting physical values from experimental data

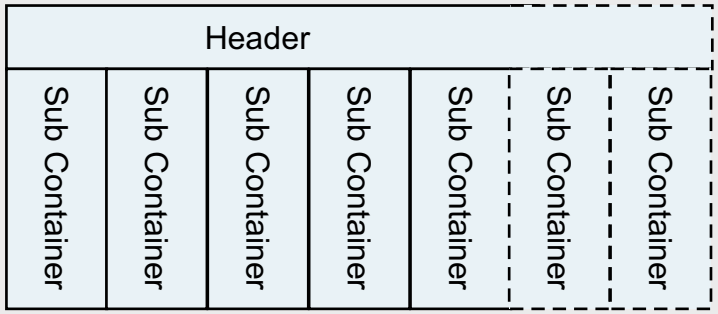
Provide common and generic analysis functionalities
for neutron scattering

Design of Data Structure

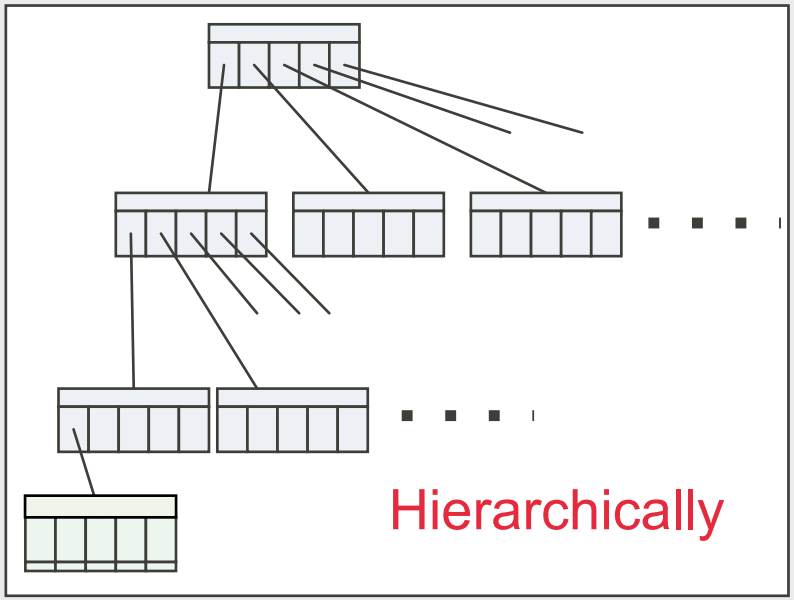
Design of data structure is one of key issues.

A sets of “simple” and “efficient” data containers are required.
Two types of class templates are provided.
Various experimental data are stored hierarchically.

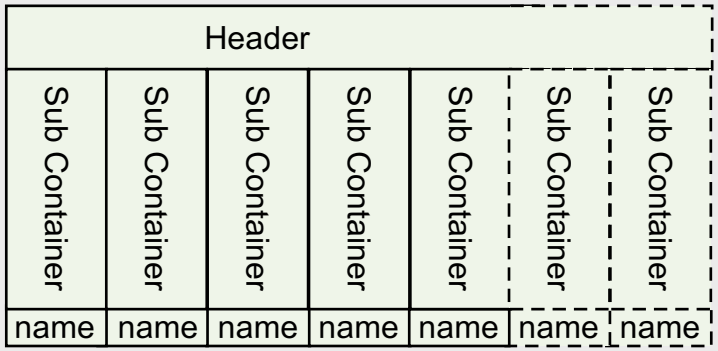
Type 1 : Container for general purpose -- consists of a Header and a set of Sub-Containers.
A header describes information about a set of Sub-Containers.
Sub-Container can store any type of object.



The number of Sub-Containers can be changed at any time.



Type 2 : Consists of Header,
a set of Sub-Containers and its names.



The sub-container is extracted by using its name-tag.