reference manual and user guide for the slacx image data workflow manager

L. A. Pellouchoud

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0.1 Introduction

The slacx software package aims to provide a fast and lean platform for exploring and processing image-like data. It was originally developed to perform analysis of x-ray diffraction patterns for ongoing projects at SLAC/SSRL. At the core of slacx is a workflow engine that uses a library of simple operations to perform data analysis, for single inputs, batches of inputs, or inputs generated in real time.

The library of operations built into slacx was designed with specific workflows in mind, and in some cases an effort was made to provide more general functionality. Some operations have been used a lot and are known to be stable, while others may introduce bugs if used in ways other than intended. In order to limit the required libraries to a few core modules, slacx defaults to a state where all operations are unavailable to the user. The user must choose which operations will be used for their workflow, and these will be imported as they are enabled. The list of enabled operations is saved in a configuration file so that they do not need to be enabled every time slacx is run.

slacx is currently written in Python, making use of the PySide Qt library bindings for GUI elements as well as data structures and threading facilities. Internally, slacx keeps track of data in a Qt-based tree, and much of the graphical part of the program involves interacting with these trees, as implemented in a Qt model-view framework.

slacx also contains a plugin that provides its functionality to xi-cam, a general-purpose synchrotron diffraction analysis software package with lots of fast and easy data analysis tools develoed by Pandolfi, et al at Lawrence Berkeley National Lab and the Camera Institute. NB: Cite and link to xi-cam here.

Some the core goals of slacx:

- Eliminate redundant development efforts
- Streamline and standardize routine data analysis
- Simplify data storage and provide large-scale analysis

The slacx developers would love to hear from you if you have wisdom, thoughts, haikus, bugs, artwork, suggestions, or limericks. Get in touch with us at slacx-developers@slac.stanford.edu.

0.2 Quick start

Minimal and usually-effective installation instructions.

0.3 Usage instructions

How to use slacx.

0.3.1 Operations

Enabling and Disabling Operations

Operation Development

0.3.2 Workflow

Building a Workflow

Execution: Serial, Batch, and Real-time

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0.3.3 Command-line Usage

0.3.4 API

Chapter 1

installation

Instructions will go here for installing slacx using the Python package installer pip, as soon as the slacx package is prepared for that. Currently, installation from pip is not implemented. Users looking to install slacx from source should build a virtual environment (optional), install the dependencies listed in section 2.1.5, and invoke the main.py module in the slacx top-level directory.

Chapter 2

system setup

Successful building of slacx depends on a few trusty, stable packages.

2.1 system dependencies

2.1.1 pip, setuptools, and wheel

pip is a Python package manager (acronym: pip Installs Python). setuptools is a Python library that supports many of the setup operations that follow. wheel is a package distribution and installation library supporting the wheel distribution standard. Users will typically want to install these together.

pip, setuptools, and wheel are installed by default on many Linux distributions and OSX, but should be upgraded. This may not be true for some Enterprise Linux (e.g. RHEL, CentOS, SL, OL) machines. Enterprise Linux users may want to see section 2.1.3. For most mainstream Linux distributions (Fedora, Ubuntu, etc.) it is suggested that the user employ the system's package manager (skip ahead to section 2.1.2).

2.1.2 pip, wheel, and setuptools for non-Enterprise Linux

The instructions differ for the various distributions. The commands listed here are copied from the web at https://packaging.python.org/. Enter the commands in a terminal, as listed for your particular distribution. If your distribution is not covered here, please consider adding its instructions to the docs and submitting a pull request.

• Fedora 21:

sudo yum upgrade python-setuptools sudo yum install python-pip python-wheel

• Fedora 22:

sudo dnf upgrade python-setuptools
sudo dnf install python-pip python-wheel

• Debian/Ubuntu:

sudo apt-get install python-setuptools python-pip python-wheel

Once pip is installed, it can be used to upgrade itself by typing:

pip install -U pip setuptools

2.1.3 pip, wheel, and setuptools for Enterprise Linux

tested on RHEL 6.8 (Santiago)

adding the EPEL repository

NOTE: You may already have connection to the EPEL repository. You can tell if you have EPEL connected by entering:

sudo yum repolist all

Look through the list, under the repo name heading, for a repo named EPEL. If you have it, skip ahead to section 2.1.3.

The easiest way to maintain pip, setuptools, and wheel is to enable the EPEL repository (Extra Packages for Enterprise Linux) for your particular distribution. The EPEL SIG (Special Interest Group) maintains rpm installers that add EPEL to RHEL's yum repository list. Begin by downloading this installer and running it with rpm.

These instructions assume you are using RHEL6, where the EPEL installer will be epel-release-latest-6.noarch.rpm. For other Enterprise Linux distributions, check the web at https://fedoraproject.org/wiki/EPEL for the correct EPEL installer file, and replace epel-release-latest-6.noarch.rpm in the following instructions with the appropriate filename.

wget https://dl.fedoraproject.org/pub/epel/epel-release-latest-6.noarch.rpm rpm -i epel-release-latest-6.noarch.rpm

These commands should enable EPEL.

installing pip from EPEL

pip is one (important) package that can be obtained from EPEL. In many cases, pip can be obtained simply by running:

sudo yum install python-pip

In some cases, the python-pip package will not be found. One possibility is that the package will have a different name in the user's specific set of repositories. The next thing to try is:

```
sudo yum install python27-python-pip
```

If this doesn't work, the user must find a package that provides pip. Try the following:

```
sudo yum whatprovides *python-pip*
```

This may return a package name like python27-python-pip-1.5.6-5.el6.noarch. Try directly installing that package:

```
sudo yum install python27-python-pip-1.5.6-5.el6.noarch
```

Once pip has been installed, it should be used to install or upgrade wheel and setuptools. With a friendly configuration, the following will work:

```
sudo pip install --upgrade setuptools
sudo pip install --upgrade wheel
```

If these throw errors, for example,

```
error while loading shared libraries: libpython2.7.so.1.0: cannot open shared object file: No such file or directory
```

the user will have to locate that shared library and add its location to their LD_LIBRARY_PATH environment variable. One way to locate the library is to ask yum to find it:

```
yum whatprovides *libpython2.7*
```

may produce something like:

```
python27-python-libs-ver.rel.arch : Runtime libraries for Python
Repo : installed
Matched from:
Filename : /path/to/libpython2.7.so.1.0
```

The search will also probably bring up some development and debugging libraries:

```
python27-python-devel-2.7.8-3.el6.x86_64 : The libraries and header files needed
    for Python development
Repo : <repo-name>
Matched from:
Filename : /opt/rh/python27/root/usr/lib64/libpython2.7.so
Filename : /opt/rh/python27/root/usr/lib64/python2.7/config/libpython2.7.so
```

and:

```
python27-python-debug-2.7.8-3.el6.x86_64 : Debug version of the Python runtime
Repo : <repo-name>
Matched from:
Filename : /opt/rh/python27/root/usr/lib64/libpython2.7_d.so
Filename : /opt/rh/python27/root/usr/lib64/libpython2.7_d.so.1.0
Filename : /opt/rh/python27/root/usr/share/systemtap/tapset/libpython2.7-debug-64.stp
Other : libpython2.7_d.so.1.0()(64bit)
```

The package that needs to be installed in each case (to get the required library) is named in the top line of each block. You might as well install any of these that are not already installed (note that python27-python-libs-ver.rel.arch is already marked as installed in this case). Install the debug and development libraries if necessary:

```
sudo yum install python27-python-debug-2.7.8-3.el6.x86_64
sudo yum install python27-python-devel-2.7.8-3.el6.x86_64
```

The path of the shared object is the line following the Filename: label. Take that line and place it in your LD_LIBRARY_PATH by adding to your shell configuration file, e.g. for ~/.bashrc:

```
echo 'export LD_LIBRARY_PATH=/dir/with/libpython/:$LD_LIBRARY_PATH' >> ~/.bashrc source ~/.bashrc
```

With this done, try again to install/upgrade setuptools and wheel:

```
sudo pip install --upgrade setuptools
sudo pip install --upgrade wheel
```

If this doesn't work, try setting up sudo to preserve your LD_LIBRARY_PATH:

```
echo "alias ldsudo='sudo LD_LIBRARY_PATH=$LD_LIBRARY_PATH'" >> ~/.bashrc export ~/.bashrc
```

Now, try again to install/upgrade setuptools and wheel, but this time use ldsudo. If it doesn't work, ask your sysadmin for help. Once these are done, some additional steps are needed to prepare the system for Qt applications. Read on, section 2.1.3

preparing PySide Qt on Linux

Since slacx is built on the Qt platform (via PySide bindings), a few more system libraries are needed. Qt itself is written in C++ and uses C extensions, so C++ and C compilers will be needed. These compilers will be used with the cross-platform cmake utility, and Qt makes extensive use of the qmake tool. This section guides you through the installation of these libraries.

1. Check for existing C and C++ compilers:

```
which cc
which c++
```

If the system has no cc or c++, find them with

```
yum whatprovides *bin/cc
yum whatprovides *bin/c++
```

A list of compiler and developer suites, for example various devtoolset versions, will come up. Take a minute to find the latest and most general version. Take note of the package name and the directory containing the binaries. Install the package and add the directory for the compiler binaries to your path.

```
sudo yum install devtoolset-<latest-versoin>-gcc.x86_64
echo 'export PATH=/opt/rh/devtoolset-4/root/usr/bin/:$PATH' >> ~/.bashrc
```

2. Repeat this process for qmake, which will come with other Qt utilities.

```
yum whatprovides *bin/qmake
sudo yum install qt-devel-4.6.2-28.el6_5.x86_64
echo 'export PATH=/usr/lib64/qt4/bin/:$PATH' >> ~/.bashrc
```

Repeat this process for cmake. For cmake, no \$PATH modifications should be needed.

```
yum whatprovides *bin/cmake
sudo yum install cmake-2.8.12.2-4.el6.x86_64
```

2.1.4 setting up a virtual environment with virtualenv

At this point, it is assumed the user has working installations of pip, wheel, and setuptools. This will be the default case for many systems. Users familiar with virtualenv may choose to skip this section.

Building software in a virtual environment is suggested as a way of sandboxing libraries that are used by other system components. After setting up pip, setuptools, and wheel (above), the installation and setup of a virtual environment is easy.

Begin by installing virtualenv:

```
sudo pip install virtualenv
```

Now, assuming you want to store the slacx virtual environment in directory <dir>, execute the following in a terminal

```
mkdir <dir>
```

virtualenv <dir>
source <dir>/bin/activate
To terminate virtualenv session:
deactivate

With the virtual environment active, Python packages can be installed without sudo and will only affect the package space of the virtual environment. Any packages installed in the virtual environment are effectively invisible once the virtual environment is turned off by calling deactivate.

2.1.5 installing python dependencies

After installing the system packages and starting a virtual environment (above), the installation of the necessary Python packages should be easy. Install each of these packages by pip install packagename>. Some of these may take a few minutes to install.

- PySide: Python Qt bindings library: Some Linux distributions may need to go through section 2.1.3 above before this installs nicely.
- QDarkStyle: A dark stylesheet for the Qt GUI.
- PyYAML: Python library for YAML serialization language

slacx is not very useful, though, without the modules that are used to operate on data. You may want to install some of the libraries that are used commonly in slacx operations:

- numpy: Python numerical computation library
- scipy: Python scientific math library
- matplotlib: Highly versatile plotting library
- PyQtGraph: Scientific visualization library built on PyQt4/PySide
- pillow: A replacement for the outdated Python Imaging Library (PIL)
- tifffile: Library for reading data from .tif image files
- fabio: Fable I/O library, parses image files from common CCD array detectors devices
- pyFAI: Fast Azimuthal Integration library for manipulating and reducing image data
- $\bullet\,$ h5py: Library for manipulating files of the fast-readable hdf5 format
- pypif: Tools for packaging data in the PIF (physical information file) format

- citrination_client: A client for communicating with a Citrination materials database
- \bullet tzlocal: Tools for interpreting time data relative to the local time zone

Chapter 3

development

This chapter covers the best practices for contributing to slacx via git (section 3.1) and instructions for developing operations for use in the slacx workflow engine (section 3.2). These instructions are intended for people who are familiar with the slacx development team and have received an invitation to work in their private repository. Public forking of the repository is not currently allowed.

3.1 contributing to slacx

The slacx repository is currently private. Request access by getting in touch with the slacx developers at slacx-developers@slac.stanford.edu. If you are looking for a long term relationship, you can send an email to join the slacx-developers listsery. Send an email to

listserv@listserv.slac.stanford.edu
with no subject and the following text in the body:

SUB SLACX-DEVELOPERS

If you want to unsubscribe, use:
UNSUB SLACX-DEVELOPERS

If you need to configure your list settings, see the ListServ manual at

Code development is currently following the "shared repository model", meaning developers have write access to the main repository. In this model, you must be careful with your edits. In particular, all coding should be done in feature branches. Never push changes directly to the master branch, and

only push to the dev branch if you are absolutely sure it's a good idea. If bad commits happen, we will roll back the problematic changes and initiate the process outlined below for pulling the new feature into dev.

The master branch is intended to be the most stable tested version, and the dev branch is for staging features that have been developed. The rest of the branches should contain features being actively developed. Once you have access, clone the repository and create your own development or feature branch. When you are satisfied, make sure your feature branch includes the latest changes to dev and either merge your feature into dev, or (if you're not fully comfortable with that), submit a pull request to review the merging of your feature with dev. Below are are step-by-step instructions for the command line and PyCharm interfaces.

If you are developing a feature that belongs in the master branch, for example if it is a stability or infrastructure or documentation fix, please always finish with a pull request.

— start here the first time you work on slacx —

- 1. Get in touch with the slacx developers to get access to the repository. See 0.1.
- 2. Clone the repository:
 - CL: git clone <REPO-URL>.
 - PyCharm: VCS ; Checkout from Version Control ; enter repository URL

This copies the remote repository (hosted online) to a local directory (on your machine). Your new directory contains the source code and a local master branch that tracks the remote master branch.

- 3. Create a dev branch that tracks the origin's dev branch.
 - CL: git checkout -b dev origin/dev.
 - PyCharm: VCS ¿ Git ¿ Branches, select origin/dev, Checkout as new local branch
- 4. Create your own feature branch.
 - CL: git branch my-feature-branch
 - PyCharm: VCS ¿ Git ¿ Branches, New branch
- 5. start here every time you work on your feature —
- 6. Check out the dev branch.
 - CL: git checkout dev
 - PyCharm: VCS ¿ Git ¿ Branches, dev -¿ origin/dev, Checkout

- 7. Pull the latest commits from the remote dev branch.
 - CL: git pull origin dev
 - PyCharm: VCS ; Git ; Pull Changes
- 8. Check out your feature branch.
 - CL: git checkout my-feature-branch
 - PyCharm: VCS ; Git ; Branches, jyourFeatureBranch;, Checkout
- 9. Rebase your feature branch onto the dev branch.
 - CL: git rebase dev
 - PyCharm: VCS ; Git ; Rebase

If you have conflicts during the rebase, due to changes in dev that disagree with changes in your feature, this step can be skipped for the moment, but these conflicts will eventually need to be cleaned up. Get help from a fellow developer, or if you are pretty sure your version of the code is better, try a pull request!

- 10. Finally, work on your feature.
- 11. After working, make sure you are still on your feature branch, then stage your edits.
 - CL: git add .
 - PyCharm: skip this step
- 12. After staging your edits, commit them with a description.
 - CL: git commit -m 'description of edits'
 - PyCharm: VCS ; Commit Changes
- Push your commits on your feature branch to the origin (remote) repository.
 - CL: git push origin my-feature-branch
 - PyCharm: VCS ¿ Git ¿ Push

Now your colleagues can see what you have done, and use your changes in their own code if they need to!

- 14. start here when you are done with your feature —
- 15. Follow steps 6 through 9 above to rebase your feature branch on dev one last time.
- 16. If you know that your changes are not likely to crash your co-workers' codes when they are merged to the dev branch, you can now merge your feature into the dev branch and push dev to the remote repository.

```
git checkout dev
git merge my-feature-branch
% mildly cautious reflection
git push origin dev
```

• PyCharm:

- VCS ¿ Git ¿ Branches, dev -¿ origin/dev, Checkout
- VCS ¿ Git ¿ Branches, ¡yourFeatureBranch¿, Merge
- mildly cautious reflection
- VCS ; Git ; Push
- 17. If you aren't 100% sure that it's safe to merge your feature into dev, submit a pull request via the online interface. Request to pull my-feature-branch into dev. The slacx development team will discuss, possibly edit, and ultimately accept your feature.
- 18. If your feature was more appropriate for the master branch, submit a pull request for the master branch.

3.2 developing operations for slacx

Developing operations for use in the slacx workflow engine is meant to be as painless as possible. A continuing effort will be made to streamline this process.

The most general description of an operation is to treat it as a black box that takes some inputs (data and parameters), performs some processing with those inputs, and produces some output (data and other features). Users can choose to build their operations in two ways.

One option is to write the function into a python class that defines names for its inputs and outputs and then stores the input and output data within objects of that class. This process is most easily understood by following the template and instructions provided in section 3.2.1 below.

Another option (not yet implemented) is to write the function into a python module that contains formatted metadata about how the function should be called, with input and output data stored in the workflow engine itself.

In either case, the user/developer writes their operation into a module somefile.py and then places this module in the slacx/slacxcore/operations/ directory. If the implementation obeys the specified format, the operation will automatically be made available to the slacx workflow manager the next time slacx is started. If the user/developer is not careful about implementing their operation, slacx may raise exceptions and exit. This could happen at startup (when the operation is read), during workflow management (when the operations is loaded with inputs), or during execution (when the operation is called upon to compute things), depending on where (if any) errors were made. Operations that are in development can be safely stored in slacx/slacxcore/operations/dmz.

3.2.1 operations as python classes

The following code block gives a minimal, commented template for developing operations as python classes. Users/developers with some programming background may find all the information they need in this template alone.

```
# Users and developers should remove all comments from this template.
# All text outside comments that is meant to be removed or replaced
# is <written within angle brackets>.
# Operations implemented as python classes
# have a common interface for communicating
# with the slacx workflow manager.
# That common interface is ensured by inheriting it
# from an abstract class called 'Operation'.
from slacxop import Operation
import optools
# Name the operation, specify inheritance (Operation)
class <OperationName>(Operation):
   # Give a brief description of the operation
   # bracketed by """triple-double-quotes"""
   """<Description of Operation>"""
   # Write an __init__() function for the Operation.
   def __init__(self):
       # Name the input and output data/parameters for your operation.
       # Format names as 'single_quotes_without_spaces'.
       input_names = ['<input_name_1>','<input_name_2>',<...>]
       output_names = ['<output_name_1>','<output_name_2>',<...>]
       # Call the __init__ method of the Operation abstract (super)class.
       # This instantiates {key:value} dictionaries of inputs and outputs,
       \hbox{\it\# which have keys generated from input\_names and output\_names}.
       # All values in the dictionary are initialized as None.
       super(Identity,self).__init__(input_names,output_names)
       # Write a free-form documentation string describing each item
       # that was named in input_names and output_names.
       self.input_doc['<input_name_1>'] = '<expectations for input 1>'
       self.input_doc['<input_name_2>'] = '<etc>'
       self.output_doc['<output_name_1>'] = '<form of output 1>'
       self.output_doc['<output_name_2>'] = '<etc>'
       # Categorize the operation. Multiple categories are acceptable.
       # Indicate subcategories with a '.' character.
       self.categories = ['<CAT1>','<CAT2>.<SUBCAT1>',<...>]
       # OPTIONAL: set default sources and types for the operation inputs.
       # This is only used for building/executing Operations in the GUI.
       # Valid sources: optools.fs_input (read input from filesystem),
       # optools.op_input (input from another operation's output),
          optools.text_input (manual text input)
       self.input_src['<input_name_1>'] = <optools.some_source>
       self.input_src['<input_name_2>'] = <etc>
       # Valid types: optools.str_type (string), optools.int_type (integer),
       # optools.float_type (floating-point number), optools.bool_type (boolean)
       self.input_type['<input_name_1>'] = <optools.some_type>
       self.input_type['<input_name_2>'] = <etc>
   # Write a run() function for this Operation.
```

```
def run(self):
    # Optional- create references in the local namespace for cleaner code.
    <inp1> = self.inputs['<input_name_1>']
    <inp2> = self.inputs['<input_name_2>']
    <etc>
    # Perform the computation
    < ... >
    # Save the output
    self.outputs['<output_name_1>'] = <computed_value_1>
    self.outputs['<output_name_2>'] = <etc>
```

3.2.2 operations as functions in a module

This functionality is not yet implemented.