
Larch Documentation

Release 0.9.7

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December 19, 2011

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Larch is a scientific data processing language that is designed to be

- easy to use for novices.
- complete enough for intermediate to advanced data processing.
- data-centric, so that arrays of data are easy to manage and use.
- easily extensible with python.

Larch is targeted at tools and algorithms for analyzing x-ray spectroscopic and scattering data, especially the sets of data collected at modern synchrotrons. It has several related target applications, all meant to be better connected through a common *macro language* for dealing with scientific data sets.

Many data collection, visualization, and analysis programs have an ad-hoc macro languages built in that allow some amount of customization, automation, scripting, and extension of the fundamental operations supported by the programs. These macro languages are rarely used in more than one program, making communication and sharing data between programs very hard.

Larch is an attempt to make a macro language that can be used for many such applications, so that the algorithms and techniques for visualization and analysis can be better shared between different programs and fields. In this respect, Larch is meant to be the foundation or framework upon which data collection, visualization, and analysis programs can be written. By having a common, extensible macro language and analysis environment, the hope is that it will be easier to make data collection, visualization, and analysis programs interact.

Larch is written in Python, has syntax that is quite closely related to Python, and makes use of many great efforts in Python, especially for scientific computing. These include numpy, scipy, and matplotlib.

The initial target application areas for Larch are

- XAFS analysis, becoming Iffeffit verversio 2
- tools for micro-XRF mapping visualization and analysis.
- quantitative XRF analysis.
- X-ray standing waves and surface scattering analysis.

Contents:

LARCH TUTORIAL

This chapter describes the Larch language and provides an introduction into processing data using Larch. An important goal of Larch is to make writing and modifying data analysis as simple as possible. The tutorial here tries to make few assumptions about your experience with scientific programming. On the other hand, Larch is a language for processing of scientific data, the expected audience is expected to have a technical background, familiarity with using programs for scientific data analysis. In addition, some understanding of the concepts of how scientific data is stored on computers and of the basics of programming.

The Larch language is implemented in and heavily based on Python. Knowledge of Python will greatly simplify learning Larch, and vice versa. This shared syntax is intentional, so that as you learn Larch, you will also be learning Python, which can be used to extend Larch. Alternatively, knowledge of Python will make Larch easy to learn. For further details on Python, including tutorials, see the Python documentation at <http://python.org/>

1.1 Getting Started

This tutorial expects that you already have Larch installed and can run either the program `larch`, basic Larch interpreter, or `larch_gui`, the enhanced GUI interpreter:

```
C:> larch
  Larch 0.9.7  M. Newville, T. Trainor (2011)
  using python 2.6.5, numpy 1.5.1
larch>
```

For Windows and Mac OS X users, executable applications will be available.

1.2 Larch as a Basic Calculator

To start with, Larch can be used as a simple calculator:

```
larch> 1 + 2
3
larch> sqrt(4.e5)
632.45553203367592
larch> sin(pi/3)
0.8660254037844386
```

You can create your own variables holding values, by assigning names to values, and then use these in calculations:

```
larch> hc = 12398.419
larch> d = 3.13556
larch> energy = (hc/(2*d)) / sin(10.0*pi/180)
```

```
larch> print energy
11385.470119348252
larch> angle = asin(hc/(10000*2*d))*180/pi
larch> print angle
11.402879992850263
```

Note that parentheses are used to group multiplication and division, and also to hold the arguments to functions like `sin`.

Variable names must start with a letter or underscore (`_`), followed by any number of letters, underscores, or numbers. You may notice that a dot (`.`) may appear to be in many variable names. We'll get to this in a later section.

1.3 Basic Data Types

As with most programming languages, Larch has several built-in data types to express different kinds of data. These include the usual integers, floating point numbers, and strings common to many programming languages. A variable name can hold any of these types (or any of the other more complex types we'll get to later), and does not need to be declared beforehand or to change its value or type. Some examples:

```
larch> a = 2
larch> b = 2.50
```

The normal `+`, `-`, `*`, and `/` operations work on numerical values for addition, subtraction, multiplication, and division. Exponentiation is signified by `**`, and modulus by `%`. Larch uses the `/` symbol for division or 'true division', giving a floating point value if needed, even if the numerator and denominator are integers, and `//` for integer or 'floor' division. Thus:

```
larch> 3 + a
5
larch> b*2
5.0
larch> 3/2
1.5
larch> 3//2
1
larch> 7 % 3
1
```

Several other operators are supported for bit manipulation.

Literal strings are created with either matched closing single or double quotes:

```
larch> s = 'a string'
larch> s2 = "a different string"
```

A string can include a `'n'` character (for newline) or `'t'` (for tab) and several other control characters as in many languages. For strings that may span over more than 1 line, a special "triple quoted" syntax is supported, so that:

```
larch> long_string = """Now is the time for all good men
.....> to come to the aid of their party"""
larch> print long_string
Now is the time for all good men
to come to the aid of their party
```

It is important to keep in mind that mixing data types in a calculation may or may not make sense to Larch. For example, a string cannot be added to an integer:


```
larch> '1' + 1
Runtime Error:
cannot concatenate 'str' and 'int' objects
<StdInput>
    '1' + 1
```

but you can add an integer and a float:

```
larch> 1 + 2.5
3.5
```

and you can multiply a string by an integer:

```
larch> 'string' * 2
'stringstring'
```

Larch has special variables for boolean or logical operations: `True` and `False`. These are actually equal to 1 and 0, respectively, but are mostly used in logical operations, which include operators `'and'`, `'or'`, and `'not'`, as well as comparison operators `'>'`, `'>='`, `'<'`, `'<='`, `'=='`, `'!='`, and `'is'`. Note that `'is'` expresses identity, which is a slightly stricter test than `'=='` (equality), and is most useful for complex objects.:

```
larch> 2 > 3
False
larch> (b > 0) and (b <= 10)
True
```

The special value `None` is used as a null value throughout Larch and Python.

Finally, Larch knows about complex numbers, using a `'j'` to indicate the imaginary part of the number:

```
larch> sin(-1)
larch> sqrt(-1)
Warning: invalid value encountered in sqrt
nan
larch> sqrt(-1+0j)
1j
larch> 1j*1j
(-1+0j)
larch> x = sin(1+1j)
larch> print x
(1.2984575814159773+0.63496391478473613j)
larch> print x.imag
0.63496391478473613
```

To be clear, all these primitive data types in Larch are derived from the corresponding Python objects, so you can consult python documentation for further details and notes.

1.4 More Complex Data Structures: Lists, Arrays, Dictionaries

Larch has many more data types built on top of the primitive types above. These are generally useful for storing collections of data, and can be built up to construct very complex structures. These are all described in some detail here. But as these are all closely related to Python objects, further details can be found in the standard Python documentation.

Here, the word “object” is used frequently. Each piece of data in Larch is a Python object, which is to say it has a value and may have specific functions that go with it.

1.4.1 Lists

A list is a sequence of other data types. The data types do not have to be the same type. A list is constructed using brackets, with commas to separate the individual:

```
larch> my_list1 = [1, 2, 3]
larch> my_list2 = [1, 'string', sqrt(7)]
```

A list can contain a list as one of its elements:

```
larch> nested_list = ['a', 'b', ['c', 'd', ['e', 'f', 'g']]]
```

You can access the elements of a list using brackets and the integer index (starting from 0):

```
larch> print my_list2[1]
'string'
larch> print nested_list[2]
['c', 'd', ['e', 'f', 'g']]
larch> print nested_list[2][0]
'c'
```

Lists are **mutable** – they can be changed, in place. To do this, you can replace an element in a list:

```
larch> my_list1[0] = 'hello'
larch> my_list1
['hello', 2, 3]
```

You can also change a list by appending to it with the ‘append’ method:

```
larch> my_list1.append('number 4, the larch')
larch> my_list1
['hello', 2, 3, 'number 4, the larch']
```

The syntax using a ‘.’ indicates a method – a function specific to that object. All lists will have an ‘append’ method, as well as several others:

- `count` – to return the number of times a particular element occurs in the list
- `extend` – to extend a list with another list
- `index` – to find the first occurrence of an element
- `insert` – to insert an element in a particular place.
- `pop` – to remove and return the last element (or other specified index).
- `remove` – remove a particular element
- `reverse` – reverse the order of elements
- `sort` – sort the elements.

Note that the methods that change the list do so *IN PLACE* and return `None`. That is, to sort a list, do:

```
larch> my_list.sort()
```

but not:

```
larch> my_list = my_list.sort() # WRONG!!
```

as that will set ‘my_list’ to `None`.

You can get the length of a list with the built-in `len()` function, and test whether a particular element is in a list with the *in* operator:

```
larch> my_list = ['a', 'b', 'c', 'd', 'e', 'f', 'g', 'h', 'i', 'j']
larch> print len(my_list)
10
larch> 'e' in my_list
True
```

You can access a sub-selection of elements with a *slice*, giving starting and ending indices between brackets, separated by a colon. Of course, the counting for a slice starts at 0. It also excludes the final index:

```
larch> my_list[1:3]
['b', 'c']
larch> my_list[:4]    # Note implied 0!
['a', 'b', 'c', 'd']
```

You can count backwards, and using `-1` is a convenient way to get the last element of a list. You can also add an optional third value to the slice for a step:

```
larch> my_list[-1]
'j'
larch> my_list[-3:]
['h', 'i', 'j']
larch> my_list[:2]    # every other element, starting at 0
['a', 'c', 'e', 'g', 'i']
larch> my_list[1::2]  # every other element, starting at 1
['b', 'd', 'f', 'h', 'j']
```

As always, consult the Python documentation for more details.

1.4.2 Tuples

Like lists, tuples are sequences of heterogeneous objects. The principle difference is that tuples are **immutable** – they cannot be changed once they are created. The syntax for tuples uses parentheses in place of brackets:

```
larch> my_tuple = (1, 'H', 'hydrogen')
```

Like lists, tuples can be indexed and sliced:

```
larch> my_tuple[:2]
(1, 'H')
larch> my_tuple[-1]
'hydrogen'
```

Due to their immutability, tuples have only a few methods (`count` and `index` with similar functionality as for list). Though they may seem less powerful than lists, tuples are actually used widely with Larch and Python, as once created a tuple has a predictable size and order to its elements. Thus, as with the example above, it can be used as a simple ordered container of data.

1.4.3 A second look at Strings

Though discussed earlier in the basic data types, strings are closely related to lists as well – they are best thought of as a sequence of characters. Like tuples, strings are actually immutable, in that you cannot change part of a string, instead you must create a new string. Strings can be indexed and sliced as with lists and tuples:

```
larch> name = 'Montaigne'
larch> name[:4]
'Mont'
```

Strings have many methods...

1.4.4 Arrays

1.4.5 Dictionaries

1.5 Conditional Execution and Control-Flow

1.6 Object and Groups

1.6.1 Objects

1.7 Reading and Writing Data

1.8 Plotting and Displaying Data

1.9 Procedures

1.10 Dealing With Errors

LANGUAGE REFERENCE

This chapter describes further details of Larch language. The most important here is the fact that Larch is closely related to Python.

Of course, Python is well-documented and much of the Python documentation can be used for Larch. Thus the discussion here focusses on the differences with Python,

2.1 Language

Larch requires Python version 2.6 or higher. Support for Python 3.X is partial, in that the core of Larch does work but is not well-tested, and

XAFS ANALYSIS WITH LARCH

One of the primary motivations for Larch was processing XAFS data.

XRF ANALYSIS WITH LARCH

X-ray Fluorescence Data can be manipulated and displayed with Larch.

DOWNLOADING AND INSTALLATION

5.1 Prerequisites

Larch requires Python version 2.6 or higher. Support for Python 3.X is partial, in that the core of Larch does work but is not well-tested, and numpy, and scipy are ported to Python 3.X. The graphical system, based on wxWidgets has not yet been ported to Python 3.X.

In addition, numpy, matplotlib, and wxPython are required. These are simply installed as standard packages on almost all platforms.

All development is done through the '**[larch github repository](https://github.com/newville/xraylarch)**'. To get a read-only copy of the latest version, use:

```
git clone http://github.com/newville/xraylarch.git
```

5.2 Installation

Installation from source on any platform is:

```
python setup.py install
```

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