



- » [NumericAndScientific](#)
- » [NumericAndScientific](#)
- » [FrontPage](#)
- » [RecentChanges](#)
- » [FindPage](#)
- » [HelpContents](#)
- » [NumericAndScientific](#)

## Page

- » Immutable Page
- » [Info](#)
- » [Attachments](#)
- » More Actions:

## User

- » [Login](#)

## Numeric and Scientific

- » [NumPy](#) - <http://www.numpy.org/> -- Numerical Python adds a fast, compact, multidimensional array facility to Python. [NumPy](#) is the successor to both Numeric and Numarray.
  - » **Deprecated:** [Numeric](#) -- Numerical Python adds a fast, compact, multidimensional array language facility to Python. (Note: superseded by [NumPy](#))
  - » **Deprecated:** [NumArray](#) - <http://stsdas.stsci.edu/numarray/index.html> -- Numarray is a reimplementation of Numeric which adds the ability to efficiently manipulate large numeric arrays in ways similar to Matlab and IDL. (Note: superseded by [NumPy](#))
- » [SciPy](#) - <http://www.scipy.org/> [SciPy](#) is an open source library of scientific tools for Python. [SciPy](#) supplements the popular [NumPy](#) module, gathering a variety of high level science and engineering modules together as a single package. [SciPy](#) includes modules for linear algebra, optimization, integration, special functions, signal and image processing, statistics, genetic algorithms, ODE solvers, and others.
- » Numba - <http://numba.pydata.org/> Numba is an open source, [NumPy](#)-aware Python compiler specifically suited to scientific codes.
- » [ad](#) is an open-source Python package for transparently performing first- and second-order automatic differentiation calculations with any of the base numeric types (int, float, complex, etc.). Utility functions designed for working with [SciPy](#) optimization routines.
- » APM Python - <http://apmonitor.com/wiki/index.php/Main/PythonApp> APMonitor is a nonlinear






programming and optimization environment with an interface to Python. The software is available as a web-service through Python libraries for the solution of large-scale mathematical programming problems.

- » **SymPy** -  <http://code.google.com/p/sympy/> **SymPy** is a symbolic manipulation package, written in pure Python. Its aim is to become a full featured CAS in Python, while keeping the code as simple as possible in order to be comprehensible and easily extensible.
- » **ALGLIB** -  <http://www.alglib.net/> - numerical analysis library in C++ and C#, with Python and **IronPython** interfaces.
- » **Python Data Analysis Library** -  <http://pandas.pydata.org/> - pandas is a library providing high-performance, easy-to-use data structures and data analysis tools for the Python .
- » **PyGSL** -  <http://pygsl.sourceforge.net/> -- This project provides a python interface for the GNU scientific library (gsl).
- » **FuncDesigner** -  <http://openopt.org/FuncDesigner> **FuncDesigner** is Python module to rapidly build functions and get their derivatives via automatic differentiation. Also you can perform integration, interpolation, interval analysis, uncertainty analysis, solve eigenvalue problems, systems of linear/non-linear/ODE equations and numerical optimization problems coded in **FuncDesigner** by **OpenOpt**.
- » **OpenOpt** -  <http://openopt.org> - a framework for numerical optimization and systems of linear/non-linear equations. Connects to dozens of solvers (some are C- or Fortran-written). Can optimize **FuncDesigner** models with automatic differentiation. Provides graphic output of convergence,  [multifactor analysis tool](#) for scientific experiments planning and some more numerical optimization "MUST HAVE" features. Also **OpenOpt** has  [Stochastic Programming and Optimization addon](#) (commercial yet, free for small-scaled academic and research purposes)
- » **SpaceFuncs** -  <http://openopt.org/SpaceFuncs> - a tool for 2D, 3D, N-dimensional geometric modeling with possibilities of parametrized calculations, numerical optimization and solving systems of geometrical equations with automatic differentiation.
- » **INLOpt** -  <http://ab-initio.mit.edu/nlopt> - another library for nonlinear optimization, including many local/global optimization algorithms written in C, with a Python interface (as well as interfaces for several other languages).
- » **jHepWork** -  <http://jwork.org/jhepwork> - a multiplatform data-analysis framework written in Java. The main programming language is Jython, a clone of Python written in Java. Contains Java libraries for numerical calculations and visualisation of scientific graphs. Contains an interactive Python prompt.
- » **ScientificPython** -  <http://dirac.cnrs-orleans.fr/ScientificPython/> -- **ScientificPython** is a collection of Python modules that are useful for scientific computing. In this collection you will find modules that cover basic geometry (vectors, tensors, transformations, vector and tensor fields), quaternions, automatic derivatives, (linear) interpolation, polynomials, elementary statistics, nonlinear least-squares fits, unit calculations, Fortran-compatible text formatting, 3D visualization via VRML, and two Tk widgets for simple line plots and 3D wireframe models. There are also interfaces to the netCDF library (portable structured binary files), to MPI (Message Passing Interface, message-based parallel programming), and to BSPLib (Bulk Synchronous Parallel programming).
- » **PyACTS**-  <http://wiki.python.org/moin/PyACTS> -- **PyACTS** is a collection of Python Modules that are very useful to Parallel Computing in a High Performance Computing environment. This packages incorporates several modules like **PyBLACS** (allows communication data for Linear Algebra), **PyPBLAS** (distributed Matrix Operations) and **PyScaLAPACK** (solve linear systems and

get the eigenvalue problems). These libraries are part of PyACTS project that provide interfaces to the ACTS Collection. Also is provided a parallel interpreter for using this package that implements message-based parallel programming using MPI.





- »  <http://pydstool.sourceforge.net> -- PyDSTool is an integrated simulation, modeling and analysis package for dynamical systems (including ODEs, DAEs, maps, and hybrid systems) and scientific data. Building on [SciPy](#) classes, the package also supports symbolic expression processing, bifurcation analysis, and enhanced arrays for "index-free" and highly contextualized scientific data manipulation. Model building tools use symbolic expression and hierarchical specification classes to ease the development and analysis of complex models. This includes automated compilation of symbolic representations of models into fast numerical code using enhanced legacy Fortran and C integrators for both stiff and non-stiff systems.
- »  [escript](https://launchpad.net/escript-finley) -  <https://launchpad.net/escript-finley> -- escript is a Python module to define and solve coupled, non-linear, time-dependent partial differential equations (PDEs). The user has to implement high-level time integration schemes and iteration schemes to reduce the problem to the solution of steady, linear systems of PDEs which are solved by a suitable PDE solver library. The current version uses the FEM solver library finley but the design is open and other libraries can be used. escript is parallelized for OpenMP and MPI. It is compatible with [NumPy](#) and VTK for visualization.
- »  [PyIMSL](http://www.roguewave.com/products/imsi-numerical-libraries/pyimsl-studio.aspx) -  <http://www.roguewave.com/products/imsi-numerical-libraries/pyimsl-studio.aspx> -- PyIMSL is a collection of Python wrappers to the mathematical and statistical algorithms in the IMSL C Numerical Library. PyIMSL offers a quality Python interface to the largest collection of portable statistical and analytical algorithms available for Python. Developers can use Python, PyIMSL and the IMSL C Library for rapid prototyping. They can then directly deploy the Python application into production or if they choose to rewrite the application in C/C++ use the same math and stats algorithms in both development environments.  [PyIMSL Studio](#) is a packaged, supported and documented development environment designed for deploying mathematics and statistics prototype models into production applications. PyIMSL Studio includes the Python language distribution and contains both open source and proprietary components that create a fully supported and documented platform for analytic prototyping and production development. PyIMSL Studio is available for download at no charge for non-commercial use or for commercial evaluation.
- » [PyGTS](http://pygts.sourceforge.net/) -  <http://pygts.sourceforge.net/> -- PyGTS is a python package used to construct, manipulate, and perform computations on 3D triangulated surfaces. It is a hand-crafted and pythonic binding for the GNU Triangulated Surface (GTS) Library ( <http://gts.sourceforge.net/>).
- » [scikit-learn](http://scikit-learn.sourceforge.net/) -  <http://scikit-learn.sourceforge.net/> -- machine learning and data mining in Python, using [NumPy](#) and [SciPy](#)
- » [mlpy](https://mlpy.fbk.eu/) -  <https://mlpy.fbk.eu/> -- Machine Learning PYthon -- high-performance Python module for Predictive Modeling.
- » [graph-tool](http://graph-tool.skewed.de) -  <http://graph-tool.skewed.de> -- A python module for efficient analysis of graphs (aka. networks), with algorithms implemented in C++ with the Boost Graph Library.
- » [spppy](http://packages.python.org/spppy/index.html) -  <http://packages.python.org/spppy/index.html> -- A sparse matrix package based on Eigen.
- » [Quandl](https://www.quandl.com/tools/python) -  <https://www.quandl.com/tools/python> -- An API package to access  <http://quandl.com> datasets, as well as upload data to Quandl.

## Multi precision math






- » MultiprecisionSoftwareDirectory (  <http://crd.lbl.gov/~dhbailey/mpdist/index.html>) - Python wrapping unknown
- » MAPM (  <http://www.tc.umn.edu/~ringx004/mapm-main.html>) - Python wrapping unknown
- » GmPy (  <http://gmpy.sourceforge.net/>) - GNU Multiple Precision library wrapping
- » mpmath -  <http://code.google.com/p/mpmath/> - mpmath is a pure Python library for arbitrary-precision floating-point arithmetic, with support for complex numbers. Implements all the transcendental functions from Python's math and cmath modules and many others.
- » clnum -  <http://calcrpnpy.sourceforge.net/clnum.html> - Class Library For Numbers wrapping

## The Grid



Grid is a type of parallel and distributed system that enables the sharing, selection, and aggregation of resources distributed across "multiple" administrative domains based on their (resources) availability, capability, performance, cost, and users' quality-of-service requirements.













- »  [PyGlobus](#) - Globus toolkit bindings for python
- »  [PEG](#) - Python Extensions for the Grid
- »  [Ganga](#) - Grid job management interface.
- »  [DIANE](#) - Python user-level middleware layer for Grids.

## Geographic Information System (GIS), Mapping, Image Processing and Analysis

- »  [Thuban](#) is a Python Interactive Geographic Data Viewer with the following features:
  - » Vector Data Support: Shapefile, PostGIS Layer, Raster Data Support: GeoTIFF Layer, Comfortable Map Navigation, Object Identification and Annotation, Legend Editor and Classification, Table Queries and Joins, Projection Support, Printing and Vector Export, API for Add-Ons (Extensions), Multi-Language Support: English, French, German, Hungarian, Italian, Russian and Spanish, User Manual (English) Multi-platform (GNU/Linux, Windows, ...). (Noli Sicad)
- »  [Python Cartographic Library](#), [OWSLib](#), [GeoJSON](#), and [Rtree](#) - packages for GIS programming and a cartographic application framework.
- »  [PySAL Python Spatial Analysis Library](#) - an open source cross-platform library of spatial analysis functions written in Python. It is intended to support the development of high level applications for spatial analysis.
- »  [sDNA](#) is freeware spatial network analysis software developed by Cardiff university, and has a  [Python API](#).

## Image analysis and visualization










- » Bokeh -  <http://bokeh.pydata.org/> - is a Python interactive visualization library for large datasets that natively uses the latest web technologies.
- » scikit-image -  <http://scikit-image.org/> - is an image processing library written in Python/Cython for use with [NumPy](#) and [SciPy](#)

- » VTK -  <http://vtk.org/> - is an open source, freely available software system for 3D computer graphics, image processing, and visualization used by thousands of researchers and developers around the world. It has a very good python interface.
- » WrapITK -  <http://code.google.com/p/wrapitk/> - interface ITK  <http://itk.org> and several languages, with a particular focus on python. ITK module used with python interpreter is particularly useful for quick and easy prototyping of image analysis procedures. Some glue classes allow to efficiently pass data to others modules like [NumPy](#) or VTK.
- » PIL -  <http://www.pythonware.com/products/pil> - Python Imaging Library provides basic image handling and processing for various image types including jpg, gif, tiff, and bmp. Reads and writes graphics files. Allows pixel-by-pixel data access and has functions for cropping and transposing an image. Also has various filters built-in.
- » matplotlib -  <http://matplotlib.sourceforge.net/> - matplotlib is a python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. matplotlib can be used in python scripts, the python and ipython shell (ala matlab or mathematica), web application servers, and six graphical user interface toolkits.
- » GR Framework -  <http://gr-framework.org/> - GR is a universal framework for cross-platform visualization applications. It offers developers a compact, portable and consistent graphics library for their programs. Applications range from publication quality 2D graphs to the representation of complex 3D scenes. GR can be used in imperative programming systems or integrated into modern object-oriented systems, in particular those based on GUI toolkits. The GR framework is especially suitable for real-time environments.
- » Plotly -  <https://plot.ly/> - is a collaborative graphing and analytics platform. The web app has an online Python sandbox - [NumPy](#) supported - and grid for data analysis. The  [Plotly graphing library](#) produces graphs that are interactive, publication quality, and browser-based. Graphs can be styled with Python or a GUI, shared, embedded, and exported.
- » Mayavi -  <http://code.enthought.com/projects/mayavi/> - application and library for interactive visualization in 3D of scientific data. High level and targeted toward the end user/application developer.
- » VisTrails -  <http://vistrails.org> - VisTrails is an open-source scientific workflow and provenance management system developed at the University of Utah that provides support for data exploration and visualization.
- » Glumpy -  <http://code.google.com/p/glumpy> - a small python library that uses OpenGL for the rapid visualization of (mainly two dimensional) numpy arrays. Not so much for nice figures for inclusion in a scientific article, more for rapid visualization of your running simulation.
- » pyqtgraph -  <http://luke.campagnola.me/code/pyqtgraph/> - Pure-python graphics and GUI library for scientific/engineering applications based on [PyQt](#) and numpy. This library provides fast plotting and image/video display, multidimensional image slicing, volumetric / isosurface rendering, interactive data manipulation tools, and a variety of Qt widgets including an editable property tree, visual programming flowchart, and gradient editor.




## Life sciences

- » Biopython -  [http://biopython.org/wiki/Main\\_Page](http://biopython.org/wiki/Main_Page) -- a set of freely available tools for biological computation and bioinformatics. It includes  [pycluster](#), a binding for the  [Cluster](#) software.
- » PyCogent -  <http://pycogent.sourceforge.net/> -- COmparative GENomic Toolkit. Another popular and extensive library for genomic biology.











- » track -  <http://xapple.github.com/track/> -- Provides easy read/write access to genomic tracks in a fashion that is independent from the underlying format. Implemented formats include: BED; WIG; GFF; GTF; BedGraph; BigWig.
- » PyChem -  <http://pychem.sf.net/> -- a cross-platform open source package for multivariate analysis, that includes a graphical user interface.
- » bx-python -  [http://bitbucket.org/james\\_taylor/bx-python/](http://bitbucket.org/james_taylor/bx-python/) -- Library and associated set of scripts to allow for rapid implementation of genome scale-analyses. Also a fundamental part of the ongoing  Galaxy and  ESPERR projects.
- » p4 -  <http://bmnh.org/~pf/p4.html> -- Python package for phylogenetics, useful for programmatic manipulation of phylogenetic data and trees, including maximum likelihood and Bayesian inference.
- » UCSF Chimera -  <http://www.cgl.ucsf.edu/chimera/> -- UCSF Chimera is a highly extensible program for interactive visualization and analysis of molecular structures and related data, including density maps, supramolecular assemblies, sequence alignments, docking results, trajectories, and conformational ensembles. High-quality images and animations can be generated. Chimera includes complete documentation and several tutorials, and can be downloaded free of charge for academic, government, non-profit, and personal use.
- » Modeller -  <http://salilab.org/modeller> -- used for homology or comparative modeling of protein three-dimensional structures. Control scripts are Python based.
- » PyMol -  <http://www.pymol.org/> -- 3D molecular viewer, suitable (and widely used) for publications and presentations. Fully scriptable in Python.




## Space Sciences

- »  Astropy aims to develop a single core package for Astronomy in Python and foster interoperability between Python astronomy packages.
- »  SunPy project is an effort to create an open-source software library for solar physics using Python.
- »  Spacepy is a set of Python-Based Tools for the Space Science Community.

## Miscellaneous

- » PyLink is an open source Python module for interfacing with the EyeLink eye tracking hardware. Find it at  PyLink
- » SimPy is an open-source discrete-event simulation package in Python. Read more at its  Homepage
- »  uncertainties is an open-source Python package for transparently performing calculations with uncertainties ( $3.14 \pm 0.01 \dots$ ).
- »  soerp is a free and open-source Python package for quickly and transparently performing calculator-style second-order error propagation (utilizes  ad for derivatives).
- »  mcerp: an open-source real-time, latin-hypercube-based Monte-Carlo alternative to uncertainty/error propagation, but isn't order specific like  soerp and  uncertainties.

## Links

- » [NumericAndScientific/Plotting](#) --
- » [NumericAndScientific/Libraries](#) -- useful libraries
- » [NumericAndScientific/Formats](#) -- modules for reading and writing various file formats
- » [NumericBooks](#)
- »  [CERN ROOT Python Services](#) -- Automatic Python/C/C++ binding
- »  [Anaconda](#) -- Free distribution with many Scientific Libraries pre-packaged.
- »  [Numfocus](#) -- Non-profit supporting [NumPy](#) stack and accessible computing for science.

## [CategoryPythonInScience](#)

NumericAndScientific (last edited 2015-08-07 07:08:08 by [ClarkZinzow](#))

- » [MoinMoin Powered](#)
- » [Python Powered](#)
- » [GPL licensed](#)
- » [Valid HTML 4.01](#)

[Unable to edit the page? See the FrontPage for instructions.](#)