Scientific computing python libraries

Below are some of the libraries which have

Scientific programming toolkits

- PyEMD : PyEMD is a Python implementation of Empirical Mode Decomposition (EMD) and its variations. One of the most popular expansion is Ensemble Empirical Mode Decomposition (EEMD), which utilises an ensemble of noise-assisted executions.
- Stable-Baselines3: Stable Baselines3 (SB3) is a set of reliable implementations of reinforcement learning algorithms in PyTorch. It is the next major version of Stable Baselines.
- Open AI gym : A toolkit for developing and comparing reinforcement learning algorithms.
- Adaptive Experimentation platform (Facebook/Meta) : Bayesian optimization and Multi-armed bandit library from Meta for performing general purpose optimization experiments.
- Optuna : Hyperparameter optimization framework to automate hyperparameter search.
- SciPy - Python modules for statistics, optimization, integration, linear algebra, etc. (Python, mostly BSD, GitHub)
- NumPy - Fundamental package needed for scientific computing with Python. (Python, BSD, GitHub)
- PETSc - Parallel solution of scientific applications modeled by PDEs. (C, 2-clause BSD, GitLab)
- DUNE Numerics - Toolbox for solving PDEs with grid-based methods. (C++, GPL 2, GitLab)

Data Visualization

- ParaView - Multi-platform data analysis and visualization application based on VTK. (C++, BSD, GitLab)
- VTK - Process images and create 3D computer graphics. (C++, BSD, GitLab)
- Mayavi - 3D scientific data visualization and plotting in Python. (Python, BSD, GitHub)
- Polyscope - Viewer and user interface for 3D geometry processing. (C++, MIT, GitHub)
- PyVista - 3D plotting and mesh analysis through a streamlined interface for VTK. (Python, MIT, GitHub)
- vedo - Library for scientific analysis and visualization of 3D objects based on VTK. (Python, MIT, GitHub)
- yt - A toolkit for analysis and visualization of volumetric data. (Python, BSD, GitHub)

Finite Elements

- FEniCS - Computing platform for solving PDEs in Python and C++. (C++/Python, LGPL 3, Bitbucket)
- libMesh - Framework for the numerical simulation of PDEs using unstructured discretizations. (C++, LGPL 2.1, GitHub)
- deal.II - Software library supporting the creation of finite element codes. (C++, LGPL 2.1, GitHub)
- Netgen/NGSolve - High performance multiphysics finite element software. (C++, LGPL 2.1, GitHub)
- Firedrake - Automated system for the solution of PDEs using the finite element method. (Python, LGPL 3, GitHub)
- MOOSE - Multiphysics Object Oriented Simulation Environment. (C++, LGPL 2.1, GitHub)
- MFEM - Free, lightweight, scalable C++ library for finite element methods. (C++, LGPL 2.1, GitHub)
- SfePy - Simple Finite Elements in Python. (Python, BSD, GitHub)
- FreeFEM - High level multiphysics-multimesh finite element language. (C++, LGPL, GitHub)
- libceed - Code for Efficient Extensible Discretizations. (C, 2-clause BSD, GitHub)

Meshing

- Gmsh - Three-dimensional finite element mesh generator with pre- and post-processing facilities. (C++, GPL, GitLab)
- pygmsh - Python interface for Gmsh. (Python, GPL 3, GitHub)
- MeshPy - Quality triangular and tetrahedral mesh generation. (Python, MIT, GitHub)
- meshio - I/O for various mesh formats, file conversion. (Python, MIT, GitHub)
- CGAL - Algorithms for computational geometry. (C++, mixed LGPL/GPL, GitHub)
- pygalmesh - Python interface for CGAL's 3D meshing capabilities. (Python, GPL 3, GitHub)
- mshr - Mesh generation component of FEniCS. (Python, GPL 3, Bitbucket)
- MOAB - Representing and evaluating mesh data. (C++, mostly LGPL 3, Bitbucket)
- NetCDF - Software libraries and data formats for array-oriented scientific data. (C/C++/Fortran/Java/Python, custom open-source license, GitHub)
- HDF5 - Data model, library, and file format for storing and managing data. (C/Fortran, BSD)
- XDMF - eXtensible Data Model and Format for data from High Performance Computing codes. (C++, GitLab)
- TetGen - Quality tetrahedral mesh generator and 3D Delaunay triangulator. (C++, AGPLv3)
- Triangle - Two-dimensional quality mesh generator and Delaunay triangulator. (C, *nonfree software*)
- optimesh - Triangular mesh smoothing. (Python, GPL 3, GitHub)

- distmesh - Simple generator for unstructured triangular and tetrahedral meshes. (MATLAB, GPL 3)
- QuadriFlow - A Scalable and Robust Method for Quadrangulation. (C++, BSD, GitHub)
- trimesh - Loading and using triangular meshes with an emphasis on watertight surfaces. (Python, MIT, GitHub)
- dmsh - Simple generator for unstructured triangular meshes, inspired by distmesh. (Python, GPL 3, GitHub)
- pmp-library - Polygon mesh processing library. (C++, MIT with Employer Disclaimer, GitHub)
- Mmg - Robust, open-source & multidisciplinary software for remeshing. (C, LGPL 3, GitHub)
- meshplex - Fast tools for simplex meshes. (Python, GPL 3, GitHub)
- TetWild - Robust Tetrahedral Meshing in the Wild. (C++, GPL 3, GitHub)
- TriWild - Robust Triangulation with Curve Constraints. (C++, MPL 2, GitHub)
- fTetWild - Fast Tetrahedral Meshing in the Wild. (C++, MPL 2, GitHub)

Sparse linear solvers

- SuperLU - Direct solution of large, sparse, nonsymmetric systems of linear equations. (C, mostly BSD, GitHub)
- KryPy - Krylov subspace methods for the solution of linear algebraic systems. (Python, MIT, GitHub)
- PyAMG - Algebraic Multigrid Solvers in Python. (Python, MIT, GitHub)
- hypre - Library of high-performance preconditioners and solvers. (C, Apache 2.0/MIT, GitHub)

Other libraries and tools

- FFTW - Discrete Fourier transforms in one or more dimensions, of arbitrary input size, real and complex. (C, GPL2, GitHub)
- Qhull - Convex hull, Delaunay triangulation, Voronoi diagram, halfspace intersection about a point, etc. (C/C++, custom open source license, GitHub)
- GSL - Random number generators, special functions, and least-squares fitting etc. (C/C++, GPL 3, Savannah)
- OpenFOAM - Free, open source CFD (computational fluid dynamics) software. (C++, GPL 3, GitHub)
- quadpy - Numerical integration (quadrature, cubature) in Python. (Python, GPL 3, GitHub)
- FiPy - Finite-volume PDE solver. (Python, custom open-source license, GitHub)
- accupy - Accurate sums and dot products for Python. (Python, GPL 3, GitHub)
- SLEPc - Scalable Library for Eigenvalue Problem Computations. (C, 2-clause BSD, GitLab)
- Chebfun - Computing with functions to about 15-digit accuracy. (MATLAB, BSD, GitHub)

- pyMOR - Model Order Reduction with Python. (Python, 2-clause BSD, GitHub)
- cvxpy - Modeling language for convex optimization problems. (Python, Apache 2.0, GitHub)
- PyWavelets - Wavelet transforms in Python. (Python, MIT, GitHub)
- NFFT - Nonequispaced fast Fourier transform. (C/MATLAB, GPL 2, GitHub)
- preCICE - Coupling library for partitioned multi-physics simulations (FSI, CHT, and more). (C++, LGPL 3, GitHub)
- orthopy - Compute orthogonal polynomials efficiently. (Python, GPL 3, GitHub)

Basic linear algebra

- BLAS - Standard building blocks for performing basic vector and matrix operations. (Fortran, public domain, GitHub)
- OpenBLAS - Optimized BLAS library based on GotoBLAS2. (C and Assembly, BSD, GitHub)
- BLIS - High-performance BLAS-like dense linear algebra libraries. (C, BSD, GitHub)
- LAPACK - Routines for solving systems of linear equations, linear least-squares, eigenvalue problems, etc. (Fortran, BSD, GitHub)
- Eigen - C++ template library for linear algebra. (C++, MPL 2, GitLab)
- Ginkgo - High-performance manycore linear algebra library, focus on sparse systems. (C++, BSD, GitHub)
- blaze - High-performance C++ math library for dense and sparse arithmetic. (C++, BSD, Bitbucket)

Communities

- SciComp StackExchange - Computational Science on the StackExchange network.
- Wolfgang Bangerth's video class - MATH 676: Finite element methods in scientific computing.
- Nick Higham's blog - Mostly on MATLAB, general computing advice.
- Nick Trefethen's Video Lectures - 36 video lectures on approximation theory/practice and scientific computing.
- John D. Cook's blog - Feats of scientific computing.
- Jack Dongarra's software list - List of freely available software for the solution of linear algebra problems.
- NA Digest - Collection of articles on topics related to numerical analysis and those who practice it.
- Gabriel Peyré on Twitter - One tweet a day on computational mathematics.