
TAO for Python

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Abstract

This document describes `tao4py`, a `Python` port to the `TAO` libraries.

`TAO` is a software package for the parallel solution of large-scale optimization problems.

`TAO` relies on `PETSc` for basic functionality such as the representation of matrices and vectors, and the solution of linear systems of equations. Thus, `tao4py` must be used together with its companion `petsc4py`.

1 Overview

TAO for Python (`tao4py`) is a `Python` package that provides convenient access to the functionality of `TAO`.

`TAO`¹ implements algorithms and tools for the numerical solution of large, sparse ...

1.1 Features

`TAO` is intended for use in large-scale application projects ...

1.2 Components

`TAO` components provide the functionality required for the parallel solutions of large-scale optimization problems.

TaoSolver Provides ...

TaoApp Provides ...

2 Tutorial

XXX To be written ... Any contribution welcome!

3 Installation

3.1 Requirements

You need to have the following software properly installed in order to build *TAO for Python*:

- Any `MPI` implementation² (e.g., `MPICH` or `Open MPI`), built with shared libraries.
- `PETSc` 3.3 or 3.2 release, built with shared libraries.
- `TAO` 2.1 or 2.0 release, built with shared libraries.
- `Python` 2.4 to 2.7 or 3.1 to 3.2³.
- `NumPy` package.
- `petsc4py` package.

¹ Lois Curfman McInnes, Jorge Moré, Todd Munson and Jason Sarich. *TAO User Manual*. ANL/MCS-TM-242 - Revision 1.10. Mathematics and Computer Science Division, Argonne National Laboratory. 2007

² Unless you have appropriately configured and built `TAO` and `PETSc` without `MPI` (configure option `--with-mpi=0`).

³ You may need to use a parallelized version of the `Python` interpreter with some `MPI-1` implementations (e.g. `MPICH1`).

3.2 Using pip or easy_install

You can use **pip** to install `tao4py` and its dependencies (`mpi4py` is optional but highly recommended):

```
$ pip install [--user] numpy mpi4py
$ pip install [--user] petsc petsc4py
$ pip install [--user] tao tao4py
```

Alternatively, you can use **easy_install** (deprecated):

```
$ easy_install [--user] tao4py
```

If you already have working PETSc and TAO builds, set environment variables `TAO_DIR` and `PETSC_DIR` (and perhaps `PETSC_ARCH` for prefix installs) to appropriate values and next use **pip**:

```
$ export TAO_DIR=/path/to/tao
$ export PETSC_DIR=/path/to/petsc
$ export PETSC_ARCH=arch-linux2-c-opt
$ pip install [--user] petsc4py tao4py
```

3.3 Using distutils

Downloading

The *TAO for Python* package is available for download at the project website generously hosted by Google Code. You can get a release tarball **curl** or **wget**.

- Using **curl**:

```
$ curl -O http://tao4py.googlecode.com/files/tao4py-X.Y.tar.gz
```

- Using **wget**:

```
$ wget http://tao4py.googlecode.com/files/tao4py-X.Y.tar.gz
```

Building

After unpacking the release tarball:

```
$ tar -zxf tao4py-X.X.X.tar.gz
$ cd tao4py-X.X.X
```

the distribution is ready for building.

Some environmental configuration is needed to inform the location of PETSc and TAO. You can set (using **setenv**, **export** or what applies to you shell or system) the environmental variables `TAO_DIR`, `PETSC_DIR`, and `PETSC_ARCH` indicating where you have built/installed TAO and PETSc:

```
$ export TAO_DIR=/usr/local/tao
$ export PETSC_DIR=/usr/local/petsc
$ export PETSC_ARCH=arch-linux2-c-opt
```

Alternatively, you can edit the file `setup.cfg` and provide the required information below the `[config]` section:

```
[config]
tao_dir    = /usr/local/tao
petsc_dir  = /usr/local/petsc
```

```
petsc_arch = arch-linux2-c-opt
...
```

Finally, you can build the distribution by typing:

```
$ python setup.py build
```

Installing

After building, the distribution is ready for installation.

You can do a site-install type:

```
$ python setup.py install
```

or, in case you need root privileges:

```
$ su -c 'python setup.py install'
```

This will install the `tao4py` package in the standard location `prefix/lib64/pythonX.Y/site-packages`.

You can also do a user-install type. There are two options depending on the target Python version.

- For Python 2.6 and up:

```
$ python setup.py install --user
```

- For Python 2.5 and below (assuming your home directory is available through the `HOME` environment variable):

```
$ python setup.py install --home=$HOME
```

and then add `$HOME/lib/python` or `$HOME/lib64/python` to your `PYTHONPATH` environment variable.