TAO for Python

Release 2.2

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Contents

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 implementation [2] (e.g., MPICH or Open MPI), built with shared libraries.

- PETSc 3.4 or 3.3 built with shared libraries.

- TAO 2.2 or 2.1 built with shared libraries.

- Python 2.4 to 2.7 or 3.1 to 3.3 [3].

- NumPy package.

- petsc4py package.

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[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 appropiatelly 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 Bitbucket. You can use **curl** or **wget** to get a release tarball.

- Using **curl**:

  ```
  $ curl -O https://bitbucket.org/dalcinl/tao4py/downloads/tao4py-X.Y.tar.gz
  ```

- Using **wget**:

  ```
  $ wget https://bitbucket.org/dalcinl/tao4py/downloads/tao4py-X.Y.tar.gz
  ```

Building

After unpacking the release tarball:

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

the distribution is ready for building.

Some environment 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 environment 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.

If you have root privileges (either by log-in as the root user of by using **sudo**) and you want to install *TAO for Python* in your system for all users, just do:

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

The previous steps will install the `tao4py` package at standard location *prefix*`/lib/python`*X.X*`/site-packages.`

If you do not have root privileges or you want to install *TAO for Python* for your private use, you have 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
  ```

  Finally, add `$HOME/lib/python` or `$HOME/lib64/python` to your `PYTHONPATH` environment variable.