Installation guide for esys-Escript

Release - 5.4
(r6850)

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July 9, 2019

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Guide to Documentation

Documentation for esys.escript comes in a number of parts. Here is a rough guide to what goes where.

install.pdf  “Installation guide for esys-Escript”: Instructions for compiling escript for your system from its source code.

cookbook.pdf  “The escript COOKBOOK”: An introduction to escript for new users from a geophysics perspective.


sphinx_api directory  Documentation for escript Python libraries.

escript_examples(.tar.gz)/(.zip)  Full example scripts referred to by other parts of the documentation.

doxygen directory  Documentation for C++ libraries (mostly only of interest for developers).
# Contents

1 Introduction 5

2 Installing from flatpak 7

3 Installing from docker 9

4 Installing from Source 11
   4.1 Parallel Technologies .......................... 11
      4.1.1 What parallel technology do I need? 11
   4.2 MacOS ...................................... 12
   4.3 Building ..................................... 12
      4.3.1 Debian .................................. 12
      4.3.2 Ubuntu .................................. 13
      4.3.3 OpenSuse ................................ 13
      4.3.4 CentOS .................................. 14
      4.3.5 Fedora .................................. 14
      4.3.6 MacOS 10.10 and later (macports) 14
      4.3.7 MacOS 10.13 and later (homebrew) 15
      4.3.8 FreeBSD ................................ 15
      4.3.9 Other Systems / Custom Builds 15
   4.4 Cleaning up ................................ 16
   4.5 Optional Extras .............................. 16
      4.5.1 Trilinos ................................ 16

A Required compiler features 17

B Trilinos 19
   B.1 Debian “stretch” configuration ................. 19
      B.1.1 Required packages ........................ 19
      B.1.2 Example configuration file ................ 19
CHAPTER
ONE

Introduction

This document describes how to install esys-Escript\(^1\) on to your computer. To learn how to use Escript please see the Cookbook, User’s guide or the API documentation.

Escript is primarily developed on Linux desktop, SGI ICE and MacOS X systems. It can be installed in two ways:

1. Binary packages – ready to run with no compilation required. These will hopefully be available in upcoming Debian and Ubuntu releases so just use your normal package manager (so you don’t need this guide).

2. From source – that is, it must be compiled for your machine. This is the topic of this guide.

See the site \url{https://answers.launchpad.net/escript-finley} for online help. Chapter 4 covers installing from source. Appendix A lists some c++ features which your compiler must support in order to compile escript. This version of escript has the option of using Trilinos in addition to our regular solvers. Appendix B covers features of Trilinos which escript needs.

\(^1\)For the rest of the document we will drop the esys-
Installing from flatpak

To install `esys.escript` on any Linux distribution using flatpak\(^1\), type

```bash
flatpak install flathub au.edu.uq.esys.escript
```

This will download and install `esys.escript` on your machine. The `esys.escript` build installed utilises both the Trilinos and PASO solver libraries, with openMP but without OPENMPI.

After flatpak has finished downloading and installing `esys.escript`, you can launch an `esys.escript` window from the menu or run `esys.escript` in a terminal with the command:

```bash
flatpak run au.edu.uq.esys.escript [other arguments to pass to escript]
```

Finally, to uninstall `esys.escript` from your machine, type

```bash
flatpak uninstall escript
```

\(^1\)For all main Linux distributions this can be installed from the repository. Otherwise, flatpak is available at `https://flathub.org/`
Installing from docker

To install an esys.escript docker container on your machine, first install docker and then type:

docker pull esysescript/esys-escript
This chapter assumes you are using a unix/posix like system (including MacOSX).

4.1 Parallel Technologies

It is likely that the computer you run esys.escript on, will have more than one processor core. Escript can make use of multiple cores [in order to solve problems more quickly] if it is told to do so, but this functionality must be enabled at compile time. Section 4.1.1 gives some rough guidelines to help you determine what you need.

There are two technologies which esys.escript can employ here.

- OpenMP – the more efficient of the two [thread level parallelism].
- MPI – Uses multiple processes (less efficient), needs less help from the compiler.

Escript is primarily tested on recent versions of the GNU and Intel suites ("g++" / "icpc"). However, it also passes our tests when compiled using “clang++”. Escript now requires compiler support for some features of the C++11 standard. See Appendix A for a list.

Our current test compilers include:

- g++ 6
- clang++ 7
- intel icpc v17

Note that:

- OpenMP will not function correctly for g++ ≤ 4.2.1 (and is not currently supported by clang).
- icpc v11 has a subtle bug involving OpenMP and C++ exception handling, so this combination should not be used.

4.1.1 What parallel technology do I need?

If you are using any version of Linux released in the past few years, then your system compiler will support OpenMP with no extra work (and give better performance); so you should use it. You will not need MPI unless your computer is some form of cluster.

If you are using BSD or MacOSX and you are just experimenting with esys.escript, then performance is probably not a major issue for you at the moment so you don’t need to use either OpenMP or MPI. This also applies if you write and polish your scripts on your computer and then send them to a cluster to execute. If in the future you find escript useful and your scripts take significant time to run, then you may want to recompile esys.escript with more options.
Note that even if your version of `esys.escript` has support for OpenMP or MPI, you will still need to tell the system to use it when you run your scripts. If you are using the `run-escript` launcher, then this is controlled by the `-t`, `-p`, and `-n` options. If not, then consult the documentation for your MPI libraries (or the compiler documentation in the case of OpenMP\(^1\)).

If you are using MacOSX, then see the next section, if not, then skip to Section 4.3.

4.2 MacOS

This release of `esys.escript` has only been tested on OSX 10.13. For this section we assume you are using either `homebrew` or `MacPorts` as a package manager\(^2\). You can of course install prerequisite software in other ways. For example, we have had some success changing the default compilers used by those systems. However this is more complicated and we do not provide a guide here.

Both of those systems require the XCode command line tools to be installed\(^3\).

4.3 Building

To simplify things for people, we have prepared `_options.py` files for a number of systems\(^4\). The options files are located in the `scons/templates` directory. We suggest that the file most relevant to your OS be copied from the templates directory to the `scons` directory and renamed to the form `XXXX_options.py` where `XXXX` should be replaced with your computer’s (host-)name. If your particular system is not in the list below, or if you want a more customised build, see Section 4.3.9 for instructions.

- Debian - 4.3.1
- Ubuntu - 4.3.2
- OpenSuse - 4.3.3
- Centos - 4.3.4
- Fedora - 4.3.5
- MacOS (macports) - 4.3.6
- MacOS (homebrew) - 4.3.7
- FreeBSD - 4.3.8

Once these are done proceed to Section 4.4 for cleanup steps.

All of these instructions assume that you have obtained the `esys.escript` source (and uncompressed it if necessary).

4.3.1 Debian

```
sudo aptitude install python-dev python-numpy libboost-python-dev libnetcdf-dev libnetcdf-cxx-legacy-dev libnetcdf-c++4-dev
sudo aptitude install scons lsb-release libboost-random-dev
sudo aptitude install python-sympy python-matplotlib python-scipy python-pyproj python-gdal
```

If you are running Wheezy, you can use:

```
sudo aptitude install gmsh
```

\(^1\)It may be enough to set the `OMP_NUM_THREADS` environment variable.

\(^2\)Note that package managers will make changes to your computer based on programs configured by other people from various places around the internet. It is important to satisfy yourself as to the security of those systems.

\(^3\)As of OSX10.9, the command `xcode-select --install` will allow you to download and install the command line tools.

\(^4\)These are correct at a time of writing but later versions of those systems may require tweaks. Also, these systems represent a cross section of possible platforms rather than meaning those systems get particular support.
to add extra meshing functionality.

Optional step
If for some reason, you wish to rebuild the documentation, you would also need the following:

```
sudo aptitude install python-sphinx doxygen python-docutils texlive
sudo aptitude install zip texlive-latex-extra latex-xcolor
```

In the source directory execute the following (substitute jessie for XXXX):

```
scons -j1 options_file=scons/templates/XXXX_options.py
```

If you wish to test your build, you can use the following:

```
scons -j1 py_tests options_file=scons/templates/XXXX_options.py
```

### 4.3.2 Ubuntu

If you have not installed `aptitude`, then substitute `apt-get` in the following.

```
sudo aptitude install python-dev python-numpy python-pyproj python-gdal
sudo aptitude install python-sympy python-matplotlib libnetcdf-c++4-dev
sudo aptitude install libboost-python-dev
sudo aptitude install scons lsb-release
```

Optional step
If for some reason, you wish to rebuild the documentation, you would also need the following:

```
sudo aptitude install python-sphinx doxygen python-docutils texlive
sudo aptitude install zip texlive-latex-extra latex-xcolor
```

In the source directory execute the following (substitute precise, quantal or raring as appropriate for XXXX):

```
scons -j1 options_file=scons/templates/XXXX_options.py
```

If you wish to test your build, you can use the following:

```
scons -j1 py_tests options_file=scons/templates/XXXX_options.py
```

### 4.3.3 OpenSuse

These instructions were prepared using openSUSE version 15.0.

Install packages from the main distribution:

```
sudo zypper in python-devel python2-numpy python2-gdal
sudo zypper in python2-scipy python2-sympy python2-matplotlib
sudo zypper in gcc gcc-c++ scons netcdf-devel
sudo zypper in libboost-python-py2_7-1_66_0-devel
sudo zypper in libboost_numpy-py2_7-1_66_0-devel
sudo zypper in libboost_iostreams1_66_0-devel
```

Now to build escript itself. In the escript source directory:

```
scons -j1 options_file=scons/templates/opensuse_options.py
```

If you wish to test your build, you can use the following:

```
scons -j1 py_tests options_file=scons/templates/opensuse_options.py
```

Now go to Section 4.4 for cleanup.
4.3.4 CentOS

These instructions were prepared using CentOS release 7 (from late 2016). The core of escript works, however some functionality is not available because the default packages for some dependencies in CentOS are too old.

Add the EPEL repository.

```bash
yum install epel-release.noarch
```

Install packages:

```bash
yum install netcdf-devel netcdf-cxx-devel gdal-python
yum install python-devel numpy scipy sympy python2-scons
yum install python-matplotlib gcc gcc-c++ boost-devel
yum install boost-python gdal-devel suitesparse-devel
```

The above packages will allow you to use most features except the `esys.downunder` inversion library. If you wish to use those it, you will need to install some additional packages.

For some coordinate transformations, `esys.downunder` can also make use of the python interface to a tool called `proj`. There does not seem to be an obvious CentOS repository for this though. If it turns out to be necessary for your particular application, the source can be downloaded.

Now to build escript itself. In the escript source directory:

```bash
scons -j1 options_file=scons/templates/centos7_0_options.py
```

Now go to Section 4.4 for cleanup.

4.3.5 Fedora

These instructions were prepared using the 28 alpha.

Install packages

```bash
yum install netcdf-cxx-devel gcc-c++ scipy
yum install sympy scons proj gdal python-matplotlib
yum install boost-devel suitesparse-devel gms2 gdal2-python
```

Now to build escript itself. In the escript source directory:

```bash
scons -j1 options_file=scons/templates/fedora_options.py
```

If you wish to test your build, you can use the following:

```bash
scons -j1 py_tests options_file=scons/templates/fedora_options.py
```

Now go to Section 4.4 for cleanup.

4.3.6 MacOS 10.10 and later (macports)

The following will install the capabilities needed for the `macports_10.10_options.py` file (later versions can use the same options file).

```bash
sudo port install scons
sudo port select --set python python27
sudo port install boost
sudo port install py27-numpy
sudo port install py27-sympy
sudo port select --set py-sympy py27-sympy
sudo port install py27-scipy
sudo port install py27-pyproj
sudo port install py27-gdal
sudo port install netcdf-cxx
sudo port install silo
```

```bash
scons -j1 options_file=scons/templates/macports_10.10options.py
```
4.3.7 MacOS 10.13 and later (homebrew)

The following will install the capabilities needed for the `homebrew_10.13_options.py` file.

```shell
brew install scons
brew install boost-python
brew install netcdf
```

There do not appear to be formulae for `sympy` or `pyproj` so if you wish to use those features, then you will need to install them separately.

```shell
scons -j1 options_file=scons/templates/homebrew_10.13_options.py
```

4.3.8 FreeBSD

At time of writing, numpy does not install correctly on FreeBSD. Since numpy is a critical dependency for esys.escript, we have been unable to test on FreeBSD.

4.3.9 Other Systems / Custom Builds

esys.escript has support for a number of optional packages. Some, like netcdf need to be enabled at compile time, while others, such as sympy and the projection packages used in esys.downunder are checked at run time. For the second type, you can install them at any time (ensuring that python can find them) and they should work. For the first type, you need to modify the options file and recompile with scons. The rest of this section deals with this.

To avoid having to specify the options file each time you run scons, copy an existing `_options.py` file from the `scons/` or `scons/templates/` directories. Put the file in the `scons` directory and name it `your-machinename_options.py`. For example: on a machine named toybox, the file would be `scons/toybox_options.py`.

Individual lines can be enabled/disabled, by removing or adding `#` (the python comment character) to the beginning of the line. For example, to enable OpenMP, change the line

```python
#openmp = True
```

to

```python
openmp = True
```

If you are using libraries which are not installed in the standard places (or have different names) you will need to change the relevant lines. A common need for this would be using a more recent version of the boost::python library. You can also change the compiler or the options passed to it by modifying the relevant lines.

**MPI**

If you wish to enable or disable MPI, or if you wish to use a different implementation of MPI, you can use the `mpi` configuration variable. You will also need to ensure that the `mpi_prefix` and `mpi_libs` variables are uncommented and set correctly. To disable MPI use, `mpi = 'none'`.

**Python3**

esys.escript works with python3 but until recently, many distributions have not distributed python3 versions of their packages. You can try it out though by modifying or adding the following variables in your options file:

```python
pythoncmd='python3'
usepython3=True
pythonlibname='whatever_your_python3_library_is_called'
```

If the name has - or other non-alpha characters, they must be replaced with underscores in the filename.
Testing

As indicated earlier, you can test your build using scons py_tests. Note however, that some features like netCDF are optional for using esys.escript, the tests will report a failure if they are missing.

4.4 Cleaning up

Once the build (and optional testing) is complete, you can remove everything except:

- bin
- esys
- lib
- doc
- CREDITS
- LICENSE
- README

The last three aren’t strictly required for operation. The doc directory is not required either but does contain examples of escript scripts.

You can run escript using path_to_escript_files/bin/run-escript. Where path_to_escript_files is replaced with the real path.

Optional step

You can add the escript bin directory to your PATH variable. The launcher will then take care of the rest of the environment.

4.5 Optional Extras

Some other packages which might be useful include:

- Lapack and UMFPACK — direct solvers (install the relevant libraries and enable them in the options file).
- support for the Silo file format (install the relevant libraries and enable them in the options file).
- VisIt — visualisation package. Can be used independently but our weipa library can make a Visit plug-in to allow direct visualisation of escript simulations.
- gmsh — meshing software used by our pycad library.
- Mayavi2 — another visualisation tool.

4.5.1 Trilinos

esys.escript now has some support for Trilinos\(^6\) solvers and preconditioners. The most significant limitation is that the current Trilinos release does not support block matrices so esys.escript can only use Trilinos solvers for single PDEs (i.e. no PDE systems).

If your distribution does not provide Trilinos packages you can build a working version from source. (See Appendix B)

\(^6\)https://trilinos.org/
Required compiler features

Building escript from source requires that your c++ compiler supports at least the following features:

- `std::complex<>`
- Variables declared with type `auto`
- Variables declared with type `decltype(T)`
- `extern template class` to prevent instantiation of templates.
- `template class classname<type>;` to force instantiation of templates
- `isnan()` is defined in the `std::` namespace

The above is not exhaustive and only lists language features which are more recent that our previous baseline of c++99 (or which we have recently begun to rely on). Note that we test on up to date versions of g++, icpc & clang++ so they should be fine.

Note that in future we may use c++14 features as well.
In order to solve PDEs with complex coefficients, escript needs to be compiled with Trilinos support. This requires that your version of Trilinos has certain features enabled. Since some precompiled distributions of Trilinos are not built with these features, you may need to compile Trilinos yourself as well.

While we can’t provide support for building Trilinos, we do list below, a configuration file which seems to work for under Debian 9 “stretch”.

B.1 Debian “stretch” configuration

B.1.1 Required packages

The following packages should be installed to attempt this build:

- cmake
- g++
- libsuitesparse-dev
- libmumps-dev
- libboost-dev
- libscotchparmetis-dev
- libmetis-dev
- libcppunit-dev

B.1.2 Example configuration file

#!/bin/bash

# Set this to the root of your Trilinos source directory.
TRILINOS_PATH=../trilinos-12.12.1-Source

# You can invoke this shell script with additional command-line arguments. They will be passed directly to CMake.
# EXTRA_ARGS=$@

rm -f CMakeCache.txt
cmake \
  -D MPI_C_COMPILER=`which mpicc` \ 
  -D MPI_CXX_COMPILER=`which mpic++` \ 
  -D MPI_Fortran_COMPILER=`which mpif77` \ 
  -D CMAKE_INSTALL_PREFIX=/usr/local/trilinos/ \ 
  -D Trilinos_ENABLE_CXX11=ON \ 
  -D Trilinos_ENABLE_Fortran=ON \ 
  -D BUILD_SHARED_LIBS=ON \ 
  -D TPL_ENABLE_BLAS=ON \ 
  -D TPL_ENABLE_LAPACK=ON \ 
  -D TPL_ENABLE_Boost=ON \ 
  -D TPL_ENABLE_Colmolmod=ON \ 
  -D TPL_ENABLE_CppUnit=ON \ 
  -D TPL_ENABLE_Matio=ON \ 
  -D TPL_ENABLE_METIS=ON \ 
  -D TPL_ENABLE_MUMPS=ON \ 
  -D TPL_ENABLE_ParMETIS=ON \ 
  -D TPL_ENABLE_Pthread=ON \ 
  -D TPL_ENABLE_SCALAPACK=ON \ 
  -D TPL_ENABLE_UMFPACK=ON \ 
  -D TPL_BLAS_INCLUDE_DIRS=/usr/include/suitesparse \ 
  -D TPL_Colmolmod_INCLUDE_DIRS=/usr/include/suitesparse \ 
  -D TPL_Colmolmod_LIBRARIES='libcholmod.so;libamd.so;libcolamd.so' \ 
  -D TPL_UMFPACK_INCLUDE_DIRS=/usr/include/suitesparse \ 
  -D TPL_SCALAPACK_LIBRARIES=/usr/lib/libscalapack-openmpi.so \ 
  -D Trilinos_ENABLE_Amesos=ON \ 
  -D Trilinos_ENABLE_Amesos2=ON \ 
  -D Trilinos_ENABLE_AztecOO=ON \ 
  -D Trilinos_ENABLE_Belos=ON \ 
  -D Trilinos_ENABLE_Itpack=ON \ 
  -D Trilinos_ENABLE_Itpack2=ON \ 
  -D Trilinos_ENABLE_Kokkos=ON \ 
  -D Trilinos_ENABLE_KokkosComplex=ON \ 
  -D Trilinos_ENABLE_Metis=ON \ 
  -D Trilinos_ENABLE_MueLu=ON \ 
  -D Trilinos_ENABLE_Teuchos=ON \ 
  -D Trilinos_ENABLE_Tpetra=ON \ 
  -D Trilinos_ENABLE_ALL_OPTIONAL_PACKAGES=ON \ 
  -D Tpetra_INST_COMPLEX_DOUBLE=ON \ 
  -D Teuchos_ENABLE_COMPLEX=ON \ 
  -D Tpetra_INST_INT_LONG=OFF \ 
  -D Tpetra_INST_INT_LONG_LONG=OFF \ 
  -D TpetraKernels_ENABLE_EXPLOSIVE_INSTANTIATION=ON \ 
  -D Trilinos_ENABLE_OpenMP=ON \ 
  -D Trilinos_ENABLE_EXPLICIT_INSTANTIATION=ON \ 
  -D KOKKOS_ENABLE_COMPILER_WARNINGS=ON \ 
  -D Amesos2_ENABLE_Basker=ON \ 
  -D Tpetra_INST_SERIAL:BOOL=ON \ 
  -D Trilinos_ENABLE_TESTS=OFF \ 
$EXTRA_ARGS \ 
$TRILINOS_PATH