

Cantera and CanteraAVBP installation tutorial

Corentin LAPEYRE

May 28, 2015

1 Who is this for?

The present document aims at describing the basic steps to compile and install Cantera and CanteraAVBP on Unix machines. The scripts and best practices match the AVBP procedures, available at www.cerfacs.fr/cantera. While Cantera scripts can be run in C, Fortran and Python, the latter is preferred for AVBP tutorials and chemistries, and the following guide aims at installing the correct python modules accordingly.

2 Dependencies

Cantera has a number of dependencies, some of which are mandatory and others optional:

Mandatory `scons`, `cython`, `python 2.7`, `numpy`

Optional `sundials`, `matplotlib`

Note that `scons` and `cython` are necessary to compile Cantera, but not to run it. Python 2.7 is industry standard and available on most systems today, and with it `numpy`.

Sundials is a nonlinear equation solver (<https://computation.llnl.gov/casc/sundials/main.html>) which enhances the convergence possibilities of Cantera, but for classical 1D flames with AVBP or even detailed chemistries, Cantera can run without it.

3 Installing it on Linux

3.1 For CERFACS users

Log into baal or asmodan :

```
$ ssh -Y baal
```

set the right PATH and PYTHONPATH :

```
$ export PYTHONPATH=
$ export PATH=/usr/bin:$PATH
```

Then the CanteraAVBP source code can be downloaded from <http://cerfacs.fr/cantera/cantera211.tar.gz>. To do so, choose an installation directory for CanteraAVBP, and copy the compressed file there. In the following, we will use the `wkdir` directory :

```
$ mkdir pathtowkdir/canteraAVBP
$ cd pathtowkdir/canteraAVBP
$ cp pathtodownloads/cantera211.tar.gz .
$ tar -xvf cantera211.tar.gz
$ cd SVNCANTERA211
```

then you can launch the build :

```
$ scons build prefix=pathtowkdir/canteraAVBP/SVNCANTERA211/
      INSTALL_DIR optimize=n blas_lapack_libs=blas,lapack
```

and finally, the install :

```
$ scons install
```

4 Installing it on Mac OS X

4.1 Dependencies

For this kind of installation, it is highly recommended to use the modern “Homebrew” package manager. It can be found at www.brew.sh. On Mac OS X, Homebrew has a single but quite large dependency: the XCode command line tools. This is the easiest way to get a proper compilation environment up and running. The installation command for these tools is:

```
$ xcode-select --install
```

which will either make a dialog box pop up to continue with the installation, or alternatively if these are already present on your computer will yield the following message:

```
xcode-select: error: command line tools are already installed,
use ``Software Update'' to install updates
```

If you do not have `cython` installed, the easiest way to install it is using `pip`. Again, if you do not have `pip`, not to worry! Simply install it using `easy_install`:

```
$ sudo easy_install pip
```

You can then use `pip` to install `cython`:

```
$ sudo pip install cython
```

4.2 Official Cantera code (OK)

brew can now finish the job for you:

```
$ brew install cantera --without-check
```

Note that the `--without-check` option is sometimes needed, as Cantera compiles successfully but some tests do not pass. Homebrew considers the passing of these tests to be mandatory, and therefore cancels the installation altogether. I do not know at this time why these tests fail, but 1D flames run well with this install.

This procedure completes the installation of the official Cantera code. The version is 2.12 at the time of writing. To use Cantera, simply source the `cantera_setup` file:

```
$ source $(which cantera_setup)
```

For more scripts, documentation, etc... please refer to the official Cantera page www.cantera.org.

4.3 CanteraAVBP, the Cantera branch with AVBP transport, analytically reduced schemes, etc ... (NOT OK)

The AVBP version of Cantera has several improvements to better integrate with the AVBP code (<http://www.cerfacs.fr/4-26334-The-AVBP-code.php>), including but not limited to:

- AVBP transport, enabling 1D flame simulation with Cantera that can be directly reproduced in AVBP;
- Analytically reduced schemes (see, for example: <http://www.engr.uconn.edu/~tlu/mechs/mechs.htm>);
- Compatibility with the `can2av` automatic conversion tool which reads a CANTERA output solution (see <http://www.cerfacs.fr/cantera/CAN2AV.php>) and translates it to an AVBP solution.

The homepage of CanteraAVBP (www.cerfacs.fr/cantera) gives further information about what is included, as well as tutorials and a chemical scheme database.

CanteraAVBP has the same dependencies as the official Cantera code. Therefore, the procedure of Sec. 4.1 can be followed to setup the correct environment for compilation. Then, the CanteraAVBP source code can be downloaded from <http://cerfacs.fr/cantera/cantera211.tar.gz>. To do so, choose an installation directory for CanteraAVBP. In the following, `~/local` is used:

```
$ mkdir -p ~/local/bundle/canteraAVBP
$ cd !$
$ wget http://cerfacs.fr/cantera/cantera211.tar.gz
```

```
$ tar xzf cantera211.tar.gz
$ cd SVNCANTERA211
```

These operations can of course be done in the Finder. `wget` is not installed by default, but it is a lightweight yet useful utility that you can get simply with `brew`:

```
$ brew install wget
```

Now setup the compilation options:

```
$ cat <<EOF >| cantera.conf
prefix = '$HOME/local'
python_package = 'new'
CC = '/usr/bin/clang'
CXX = '/usr/bin/clang++'
f90_interface = 'n'
python_compiler = '/usr/bin/clang++ -stdlib = libc++'
EOF
```

Now, the code can be compiled using `scons`:

```
$ scon build
```

Here again, `scons` is not installed by default, but you can get it with `brew`:

```
$ brew install scon
```

References