Installing CEA on an Intel Mac

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April 20, 2012

1 Introduction

Chemical Equilibrium with Applications (CEA) is a computer program published by NASA Glenn with the purpose of calculating chemical equilibrium product concentrations from any set of reactants and determining thermodynamic and transport properties for the product mixture [1].

The reason that you're reading this document is that you'd like to install CEA on an Intel-based Macintosh computer, which is an unfortunately complicated procedure. The process presented in this document was compiled from the notes of Professor Brian Cantwell, Siina Haapanen, Minna Chao, Ashley Chandler, from the help of Matthew Giarra, and from references [2] and [3]. It has been tested in OS X 10.6.4 (Snow Leopard) by the author, and in OS X 10.5 (Leopard) by Rosalind Beckwith.

2 Dramatis Personae

The characters involved in this play include:

CEA - a Fortran program coupled with a Java user interface

gfortran - GNU compiler for Fortran programs (free alternative to UNIX's f77)

gcc - GNU compiler collection - a set of compilers for various programming languages

terminal - OS X's porthole to the UNIX command line

XCode Tools - a set of tools for developing software on OS X

root - the "super-user" on a UNIX machine

emacs - a UNIX text editing program

3 Terminal

There are many ways of getting to the UNIX command line which is buried under the shiny beautiful surface that is the OS X user interface. One of the simpler, no-frills methods is using the program Terminal which is located in the utilities folder inside of the applications folder.

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This opens the `bash` shell by default, and if it's not you can switch back through Terminal's preferences menu (if it's running `bash` already, it will say so at the top of the window):

Open Terminal preferences, and find the option under "startup" that will automatically enter a command each time Terminal is opened. Make this command `/bin/bash` . Alternatively, for a single window you can just type the command `bash` to change it for that window only.

4 XCode Tools

You will need to install XCode Tools to obtain the `gcc`. While XCode Tools comes with OS X, it is not installed by default. This can be done by popping the OS X DVD into your computer, navigating to "Optional Installs" and starting the XCode Tools installer.

It can also be obtained online via Apple's website:

http://developer.apple.com/TOOLS/Xcode/

To download it from the site, Apple does require that you sign up for an Apple Developer Connection account, but it's free and is comparable to the hassle of finding your OS X install DVD anyway. You can also log in using a normal Apple ID if you have one, and they'll only ask you a few more probing questions.

5 gfortran

To make CEA function, you need to recompile some of the Fortran programs. To do that, you of course need some way of compiling Fortran programs! With XCode Tools, you've installed `gcc`, a compiler for a wide range of programming languages that by default doesn't include Fortran. To obtain a Fortran compiler, `gfortran`, you must head to

`http://hpc.sourceforge.net/`

Where you can find under the heading "**GCC 4.6 (auto-vectorizing gcc with openmp)**" the links for downloading the gfortran files, specific to either Leopard or Snow Leopard. Make sure you just download the gfortran package, and not the whole gcc package. Once you've downloaded the gfortran package, you'll need to move it to somewhere useful, unzip it, and install it.

Depending on the setup of your computer and user profile, you may need to switch to the root user of your system in order to complete some of the following commands. To switch to root, simply type in the terminal window `su root`, and then enter the appropriate password.

If you are not the owner of your computer, you should probably contact the owner before trying to continue. If you are the owner of the computer and you don't know the root password, first try your own user's password. If that doesn't work, the root password may never have been set. You can set it using the command `sudo passwd root`. Then enter your own password, and set the root password to whatever you'd like.

Continuing with the installation, first you'll need to make a directory in which to put `gfortran`:

```
mkdir /usr/local/src/gfortran
```

However, if `/usr/local/src` doesn't exist (you'll get an error when you try to type the above command), you'll first have to make it:

```
mkdir /usr/local/src
```

Then to move the downloaded file to the target directory, first navigate to the location where it was downloaded, and then use the following commands (these commands are for the Snow Leopard file, if you're using Leopard, just replace `snwleo` with `leopard`):

```
cp gfortran-snwleo-intel-bin.tar /usr/local/src/gfortran
```

Now move the working directory to that folder:

```
cd /usr/local/src/gfortran
```

and then to install it:

```
tar -xvf gfortran-snwleo-intel-bin.tar -C /
```

to test if it installed correctly, simply type `gfortran -v` . If it returns something similar to:

```
Using built-in specs.
COLLECT_GCC=gfortran
COLLECT_LTO_WRAPPER=/usr/local/libexec/gcc/x86_64-apple-darwin10/4.6.0/lto-wrapper
Target: x86_64-apple-darwin10
Configured with: ../gcc-4.6-20100703/configure --enable-languages=fortran --host=x86_64-apple
Thread model: posix
gcc version 4.6.0 20100703 (experimental) (GCC)
```

then you're all set (some of it will be different depending on your computer and version of OS X).

If it returns `command not found`, then something's wrong. One possible reason is that the installed directory isn't in the normal search path, so your computer isn't seeing it. To see if this is the case, type: `echo $PATH` , and look at the list of directories that it outputs. If `/usr/local/bin` was not one of the directories, then you need to add it to the path. This can be done by typing

```
echo 'export PATH=/usr/local/bin:$PATH' ≫ /.profile
```

(be very careful with the spaces - there's only one after the ≫) and then closing your terminal window, quitting the program, and then restarting terminal with a new window. Type `echo $PATH` to make sure it worked. If this also didn't work, see the notes at the end of the next section about the alternate method for updating the `PATH` variable.

If for whatever reason you decide to uninstall gfortran, go to the directory that you installed it *from* (ie `cd /usr/local/src/gfortran/`) and run this code:

```
tar -tf gfortranfile | sort -r | (cd /; xargs -t -n 1 rm -d)
```

6 CEA Files

To download the CEA files themselves, go to the following page on NASA Glenn's site:

http://www.grc.nasa.gov/WWW/CEAWeb/ceaguiDownload-unix.htm

From here, download the following three files:

- CEAgui JAR (CEAgui-jar.tar.Z)
- CEA+Fortran Package (CEA+Fortran.tar.Z)
- CEAexec Package (CEAexec-mac.tar.Z)

Make a new directory and save all of these files in it This will be where CEA is installed, so place it wherever you'd like the final program to be. Then, open a terminal window and navigate to the folder where the files are, and use the following commands to uncompress the files (do *not* use a program like Stuffit Expander):

```
zcat CEA+Fortran.tar.Z | tar xvf -
zcat CEAexec-mac.tar.Z | tar xvf -
zcat CEAgui-jar.tar.Z | tar xvf -
```

When you're finished, you should have the following six files in this folder: `CEAgui.jar, thermo.lib, trans.lib, syntax, b1b2b3, FCEA2`. If not all six are present, check that you have correctly downloaded and unpacked all three packages. Now, the permissions of several files have to be changed. This can be done using the following commands:

```
chmod a+x b1b2b3
chmod a+x syntax
chmod a+x FCEA2
chmod a+x runCEA.sh
```

Finally the environment variable `PATH` must be changed to include the CEA installation directory. Do this by typing:

```
echo 'export PATH=/directory/where/CEA/is:$PATH' ≫  /.profile
```

And then quitting and restarting terminal (make sure you replace `/directory/where/CEA/is` with the actual directory!). Type `echo $PATH` and make sure that your CEA installation directory is on the list.

For some people this method of updating `PATH` does not work, and while I have been unable to determine the reason, there is another way to do it. It involves opening a text document that contains a list of directories, and then adding the CEA directory to that list. The text editor of choice is `emacs` , and opening the file into it can be done by typing (note that you will need to be logged in as root for this step):

```
emacs /etc/paths
```

Now, navigate to the bottom of the file with the arrow keys, and then add on the next line the

directory where CEA is installed. For example, once I added the directory to my `PATH` file, it looked like this:

```
/usr/bin
/bin/
/usr/sbin
/sbin
/usr/local/bin
/jez/school/stanford/cea stuff/CEA
```

To exit `emacs` hit `ctrl-x` and then `ctrl-c` . When it asks you if you want to save the file, type `y` .

7 Update CEA Files

Now, some of the CEA Fortran files need to be recompiled. To do that, move to the CEA installation directory and type the following code:

```
gfortran cea2.f
mv a.out FCEA2
gfortran b1b2b3.f
mv a.out b1b2b3
gfortran syntax.f
mv a.out syntax
```

If during this process you get a long string of warning messages about `feature deleted: goto ...` it's bogus and safe to ignore. Now you should have new executable files, but you'll still need to get new library files. To do that, type:

```
FCEA2
trans
FCEA2
thermo
FCEA2
cea2
```

Note that each time you type `FCEA2` you should get a statement asking for the input filename. You should now be all set. To try it out, type `./runCEA.sh` in the CEA installation directory, and try loading an example file and executing it.

8 Troubleshooting

This section is still in progress. If you have any problems, let me know and I'll add it here.

There are many ways to go wrong installing this software, so here is a list of common errors and what they mean:

File not found! Runtime.getRuntime().exec(b1b2b3) not complete due to the missing thermo.lib or trans.lib or BAD data! This means that you didn't update the CEA files correctly. Make sure that you didn't get any error messages when completing that part of the installation.

ERROR: Missing Fortran Executable File: FCEA2.exe or FCEA2 ! Please Exit!
This means that the PATH environment variable doesn't include the CEA installation directory.

```
as: assembler (/usr/bin/../libexec/gcc/darwin/x86_64/as or
/usr/bin/../local/libexec/gcc/darwin/x86_64/as) for architecture x86_64 not installed

 as: no assemblers installed
```

I don't entirely know the details behind this error, but it seems to be related to the installation of the `gcc`. Reinstalling XCode Tools and then proceeding with the installation from there has solved this error in the past.

References

[1] http://www.grc.nasa.gov/WWW/CEAWeb/ceaWhat.htm

[2] http://hpc.sourceforge.net/

[3] http://www.webmo.net/support/fortran_osx.html