R.E.D. FOR MAC OS X INSTALL GUIDE

by Thomas A. D. Patko – California State University Long Beach, USA

REQUIRES R.E.D.-III.2 or HIGHER

The notes below may not be the only way to get the R.E.D. program working on your Mac, but they are the way that I got it going. If you have any corrections or alternative methodology that you wish to suggest, it is encouraged that you share your thoughts with the R.E.D. development team by posting on the q4md, CCL or AMBER mailing lists so that others may benefit from your feedback. If you should have any questions about the instructions in this guide, it is also encouraged that you post to these same lists for assistance. R.E.D.-III.2 and R.E.D.-III.3 have been tested on Leopard (10.5.8) and Snow Leopard (10.6.1).

INSTALL ALL OF THE DEVELOPER DEPENDENCIES

You will need to download and install a current version of XCode (see link below). There is no cost associated with this except that you will need to register with Apple and give a brief description of your planned usage of the developer tools. All of the developer tools to compile the needed dependencies (namely the RESP program) are provided with the XCode download (such as gcc, g++, etc…), with the exception of the necessary fortran compiler, which is addressed in the next section. Note that the default shell for Leopard and Snow Leopard is BASH, and all instructions in this guide will assume that you are using this default shell.

http://developer.apple.com/technology/xcode.html

You will also need to download and install a current version of the fortran compiler "gfortran". Simply select the appropriate download for your OS architecture (PPC or Intel). You do NOT need to download the XCode plugin (although you can if you wish).

http://gcc.gnu.org/wiki/GFortranBinaries

INSTALL THE *AB INITIO* SOFTWARE

Currently GAMESS-US, PC GAMESS / Firefly, and Gaussian are supported *ab initio* packages for R.E.D. on the Apple Mac platform. Although all three packages are supported, only the first two of these were actually tested for proper function, as I do not have a Gaussian for Intel Mac license. If anyone else out there that has a valid Gaussian for Intel Mac license and wishes to confirm nominal function with R.E.D.-III.2 or higher on the

Mac platform it would be appreciated. Find below links to download each of these along with some comments that will be useful configuration tips to make each of these packages to work with R.E.D.

GAMESS-US for Mac

You will need to go to the following URL (see link below) and agree to the license agreement and then request the appropriate download.

http://www.msg.chem.iastate.edu/GAMESS/download/register/

The GAMESS-US package is provided free of charge and bound by the license terms as described. If you are a new user it may take some time for your e-mail address to be approved. Although you can compile GAMESS from source on the Mac platform, for all computations conducted by R.E.D. you can instead simply use the pre-compiled binaries that are offered (for these job types there will most likely be little or no improvement for speed). To do this, simply check the "GAMESS version April 11, 2008 R1 for Apple MacOS X" as the "Pre-compiled Binary Distributions" that you wish to receive (or the equivalent most recent version).

When you receive your download e-mail you will be offered three versions of GAMESS for your Mac:

gamess-OSX-Current.tar.gz
(This is the version for all PPC Mac machines)

gamess-OSX-Current.x86.tar.gz
(This is the version of some early Mac Intel machines using the Core Duo architecture)

gamess-OSX-Current.x86-64.tar.gz
(This is the version FOR MOST CURRENT Mac Intel machines using the Core 2 architecture)

Just download and open the correct version and pick a reasonable location on your Mac to install it. If multiple users will be using this same program be sure to set the directory and file permissions to be 755 or higher (they are set more strict by default when you download it which is fine for use by just a single user). Wherever you chose to put the GAMESS folder you will need to add the absolute path of that directory to your PATH in order for R.E.D. to be able to use it. **Look at Appendix 1 for some notes about graphical modes to edit your shell environmental variables if you do not wish to do it from a command line.** You will need to append your

PATH environmental variables so that R.E.D. can find your GAMESS executables. I chose to install GAMESS into my user account (*i. e.* "tpatko") and consequently I added in my ".profile" file:

export PATH=$PATH:/Users/tpatko/gamess

You will need to add all of the required environmental variables to your ".profile" (see Appendix 1). Note that "tpatko" would be replaced by whatever your user account actually is under Mac OS or where it is that you chose to place your working GAMESS binary installation directory.

All of your scratch directory variables are set in the actual "rungms" script. Please review the RED-II manual (see the documentation section of the R.E.D. website) and the GAMESS documentation (many useful notes are written directly in the "rungms" script itself) for further details about how to properly configure your "rungms" script. You should only need to modify the following line from your "rungms" script to ensure compatibility with R.E.D.:

setenv PUNCH $USERSCR/$JOB.dat
should become
setenv PUNCH $SCR/$JOB.dat

Be sure that you have successfully launch GAMESS jobs BEFORE trying to interface this package with R.E.D. Note that the scratch directory specified in your "rungms" script must exist and be empty before a R.E.D. job is called, and you obviously must have read/write permissions to this directory.

PC GAMESS / Firefly for Mac

There is a web page dedicated to installing PC GAMESS / Firefly on the Intel Mac platform. Simply follow the directions on this page, and make sure that all of the tests and benchmarks pass.

http://classic.chem.msu.su/gran/gamess/macosx.html

You will have to append the following environmental variables to your ".profile" so that R.E.D. can find your PC GAMESS / Firefly for Mac installation and know the scratch directory that you wish to use (the scratch directory path indicated below I just an example as any suitable directory may be selected).

export PATH=$PATH:/Applications/PC-GAMESS-FIREFLY-MAC
export PCGAMESS_SCRDIR=/tmp/firefly

Look at Appendix 1 for some notes about graphical modes to edit your shell environmental variables if you do not wish to do it from a command line.

By default, DARWINE dependency path is hard coded into R.E.D. since the default PC GAMESS / Firefly installation also assume this hard coded path (just install DARWINE into the normal /Applications folder and you will be fine). You can set the PCGAMESS_SCRDIR path to be anything that you wish. Using the export environmental variable settings described should work for most users assuming that you have performed a default install of PC GAMESS / Firefly for Mac. If you have changed the location of the DARWINE dependency or the PC GAMESS / Firefly installation path from the defaults, you will need to make adjustments accordingly. The default install of PC GAMESS / Firefly should be fine for most users and it is assumed that this is the case throughout the remainder of this guide. Note that the scratch directory MUST exist and be empty prior to launching any R.E.D. job and you must obviously have read/write permissions to this directory.

The easiest way to setup the example PC GAMESS scratch directory from a terminal is:

cd /tmp
mkdir firefly

Be sure that you have successfully launch PC GAMESS / Firefly jobs from the drag and drop apps and a command line BEFORE trying to interface this package with R.E.D.

Gaussian for Intel Mac

In principle you should be able to interface R.E.D. with Gaussian for Intel Mac distribution as it should function exactly as any typical Linux/UNIX version of Gaussian. Please perform the standard (recommended) installation of Gaussian as discussed in the Gaussian for Intel Mac documentation. As mentioned at the beginning of this guide, Gaussian was not tested as I do not have a License for Gaussian for Intel Mac but in principle this should work just fine. You will need to configure your Gaussian scratch directory, picking some suitable location (one example is provided below).

export GAUSS_SCRDIR=/tmp/gaussian

Look at Appendix 1 for some notes about graphical modes to edit your shell environmental variables if you do not wish to do it from a command line.

Reports from users with a valid Gaussian for Intel Mac license that have been successfully able to interface this program with R.E.D.-III.2 or above on Leopard or Snow Leopard would be appreciated (along with any tips if appropriate).

INSTALL AMBERTOOLS

Strictly speaking you can find the RESP program from sources other than AMBERTOOLS, although it is freely available from this source, and has some nice convenient instructions on how to configure and compile the AMBERTOOLS which includes the necessary RESP program. Once again, you will need to add some environmental variables to your user profile (namely $AMBERHOME and to append your path to include the absolute path to where you built your AMBERTOOLS binaries). The default configure (./configure_at gcc) and make instructions (make -f Makefile_at) as described in the README_at file should work fine on both Leopard and Snow Leopard and will produce a working RESP binary for R.E.D.

http://ambermd.org/AmberTools-get.html

Once again you will need to setup your environmental variables so that AMBERTOOLS (and most importantly in our case RESP) will work correctly. If you are comfortable setting up environmental variables on a Linux/UNIX system, just do this as usual. If not, please consult Appendix 1. I chose the following locations for the installation, although any valid location should do just fine:

export AMBERHOME=/Applications/amber10
export PATH=$PATH:$AMBERHOME/exe

CONFIGURE R.E.D.

You will need to be sure to have R.E.D.-III.2 or higher to ensure that it works properly on the Mac Intel platform. Follow the instructions on how to setup R.E.D. contained in the download. Once completed, you should be able to run the "HowTo" provided in the download. If these jobs complete correctly, you will be ready to run your own charge derivation on your Mac!

http://q4md-forcefieldtools.org/RED/

R.E.D. III.2 and III.3 were tested on Leopard and Snow Leopard using the pre-compiled binaries of GAMESS version April 11, 2008 R1 for Mac OS X (64-bit) and PC GAMESS / Firefly version 7.1.F for Mac. More recent versions of both *ab initio* programs should also work just fine.

RUNNING X RED

X RED-III.2 and X RED-III.3 have been successfully tested on Leopard and Snow Leopard with GAMESS and PC GAMESS / Firefly (versions as previously described). All function is nominal. Please consult the main RED documentation for details about using X RED, although the use is rather intuitive. Simply call X RED from a terminal shell (assuming that your current working directory is the same as the location of the XRED-III.2.tcl or XRED-III.3.tcl file) by calling "wish X RED-III.x.tcl". You should ensure that RED-III.x works from a command line BEFORE trying to use X RED!

APPENDIX 1

To modify your path and other environmental variables is it often convenient to use TinkerTool (to view hidden files) and TextWrangler (to edit text files). Further down in this Appendix, links for downloading these two free programs are provided. For most users, your profile can be found in the hidden ".profile" file in the root of your user directory (when using the system default BASH shell terminal).

Download the free utility TinkerTool

The Mac Finder does not show invisible files (including important system configuration files that begin with ".") and many system file folders. One of the folders that is not displayed is the temporary folder (/tmp) which is important for cleaning up jobs that do not exit gracefully. To view this and folders not normally visible under the normal Apple Finder you can use TinkerTool that allows you to toggle between viewing hidden (invisible) and system files and folders and returning back to the default hidden status. Just simply click on the Show hidden and system files checkbox under the Finder tab and click on relaunch Finder button. To disable viewing hidden and invisible files just uncheck the same checkbox and relaunch Finder again. You can download TinkerTool at:

http://www.bresink.de/osx/TinkerTool.html

Download the free utility TextWrangler

You will want to have a text editor that supports UNIX, Mac and Windows text files. The TextEdit program that is found in the main /Applications directory is not suitable for the purpose of viewing text output (such as those from Firefly jobs while they are running) if the file is being written to as you view it (no auto-refresh). In addition, the TextEdit program is not the best choice to view large text files. As such the Free program TextWrangler that is suitable for both of these purposes and has been made a dependency that must be meet prior to running the DMG installer. When you run the graphical dependency test application, a browser will automatically be opened to the download website page for TextWrangler and it is reproduced below for your convenience.

http://www.barebones.com/products/textwrangler/

I would recommend installing TextWrangler into the typical /Applications folder (default install). All further details will assume this standard installation location.

Once TinkerTool and TextWrangler are installed on your system, it is easy to find and edit any "hidden" files on your system including your user configuration file (the default terminal shell for Tiger and Leopard). Simply look in your /Users/$USER directory (where $USER is your username) and you will see your ".profile" confirmation file.

Editing your ".profile" user configuration file for the BASH shell

You will need to edit this file several times along this procedure to get everything working for R.E.D. Navigate to the root of your user account (/Users/YOURUSERNAME/). There you should see a folder called ".profile". If you do not see this file you will need to create it. To create it if it does not exist just open a terminal shell (/Applications/Utilities/Terminal.app) and type the following:

```
cd ~
touch .profile
```

You can then open this empty ".profile" text file with TextWrangler or from your command line terminal with "vi" (if you are not familiar with the command line "vi" editor you can search on Google for guides on how to use "vi"). Editing this hidden ".profile" file in the root of your user account can be done with either a graphical text editor was as Text Wrangler or from a command line.

A typical set of environmental variable exports to be added to get GAMESS and PC GAMESS / Firefly working with R.E.D. would be ("tpatko" would be replaced by whatever your user account actually is under MacOS):

To interface PC GAMESS / Firefly with R.E.D. you should have something like this in your user profile:

```
export PATH=$PATH:/Applications/PC-GAMESS-FIREFLY-MAC
export PCGAMESS_SCRDIR=/tmp/firefly
```

Note: The binary path for PC GAMESS / Firefly is the default (should be fine unless you changed it). The scratch directory can be anywhere you wish to use (preferably a different drive than our OS drive with a lot of free disk space).

To interface GAMESS-US with R.E.D. you should have something like this in your user profile:

```
export PATH=$PATH:/Users/tpatko/gamess
```

To interface Gaussian with R.E.D. you should have something like this in your user profile:

```
export GAUSS_SCRDIR=/tmp/Gaussian
```

NOTE: You may need additional environmental variables to get your Gaussian for Intel Mac installation working properly. At minimum the GAUSS_SCRDIR variable is required by R.E.D. but it is possible that the actual Gaussian binaries required additional environmental variables to be set. Please consult the Gaussian documentation for additional details.

To configure your user profile to find the RESP binary:

```
export AMBERHOME=/Applications/amber10
export PATH=$PATH:$AMBERHOME/exe
```

Obviously, you will need to adjust the exact paths to reflect your particular installations and the above are simply provided as examples.

IMPORTANT NOTE ABOUT ENVIRONMENTAL VARIABLES

Recall that changes made in your ".profile" file will not take effect in your shell until your start a new session and/or you logoff/login again. Alternatively, you can simply execute the export commands manually from a command line each time you wish to set them (or update them for testing, etc…) or simply source your ".profile" (this will update all environmental variables in your ".profile"). To source your ".profile" simply do the following from a command line terminal:

```
cd ~
source .profile
```

Mac specific installation notes and usage guide

Thomas Patko, Dept. of Chemistry & Biochemistry, California State University, Long Beach, USA

Last Revised October 1st, 2009