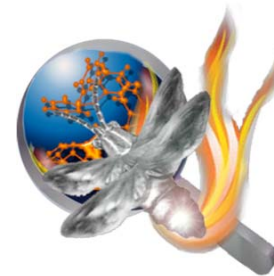


QUICK START AND USAGE GUIDE
FOR INSTALLING AND RUNNING
PC-GAMESS / FIREFLY UNDER MAC OS X
(Tested on Tiger & Leopard)



FOR MAC INTEL MACHINES ONLY!!

There is no PPC platform version available (nor will there be one in the future).

Thank you for your interest to the PC-GAMESS/Firefly package! Please follow the quick start guide below to get your installation up and running. Please note that this quick start guide is not intended as a replacement for the more complete install and usage guide that will give more extensive and complete information about the installation and usage of PC-GAMESS/Firefly on Mac. If you should encounter any problems with the quick start guide, please refer to this more complete document. In addition, this guide assumes are reasonably good working knowledge of the current documentation and that the users reading this guide only need the specifics of how to run the Mac implementation. If this is not the case, please review the relevant posted documentation as necessary and appropriate.

To view the most current version of PC-GAMESS/Firefly, you will want to visit the official project homepage at: <http://classic.chem.msu.su/gran/gamesess/index.html>

There is also a Mac specific page posted at <http://classic.chem.msu.su/gran/gamesess/macosex.html> although you should always also visit the main home page to find out about major project announcements, updated and general points of interest for all PC-GAMESS/Firefly users.

Lastly, there is also a Mac beta webpage located at http://classic.chem.msu.su/gran/gamesess/macosex_beta.html that may contain newer versions that are provided on the main public release website. Please note that anything from the beta website may or may not work as expected and is intended for the adventurous in spirit and those requiring a particular new feature that is not yet available in the last public release.

STAGE 1: Getting the Dependencies Installed

Download the application that will determine what dependencies need to be installed to ensure that your computer is ready to run PC-GAMESS / Firefly for Mac. The download URL is:

<http://classic.chem.msu.su/gran/gamess/macosex/TEST-FIREFLY-DEPENDENCIES.zip>

Just double click on the downloaded .zip archive and a folder called TEST-FIREFLY-DEPENDENCIES will be created. Just double click on the Mac application “CHECK FIREFLY DEPENDENCIES RUN ME FIRST” inside this folder. If your computer already has all of the dependencies (helper applications required for normal operation) then you will see this returned:

Testing the required dependencies for PC-GAMESS / Firefly to run on your Apple Macintosh Computer:

X11 is installed on this system

Darwine is installed on this system

TextWrangler is installed on this system

End of Dependency Testing.

ALL TESTS SUCCESSFULLY PASSED.

Go ahead and run the Firefly DMG Installer (Install Code Required!!)

TO OBTAIN INSTALL CODE FOR THE Firefly DMG INSTALLER PLEASE SEND REGISTRATION E-MAIL REQUEST TO gran@classic.chem.msu.su WITH THE REQUESTED INFORMATION (SEE [Registration_email_template.txt](#) for Details)

If your computer is missing any of the dependencies, a Safari window will pop-up that provides a download link to the required programs. All dependencies for PC-GAMESS / Firefly to run on your Mac are FREE software (either open source or available for use without registration or cost to the end user). Please do not proceed to the next Stage until you computer passes the dependency test and returns the text as shown above.

STAGE 2: Getting a License code to run the Mac DMG installer

First, carefully read the contents of the enclosed "License.pdf" file included with your dependency testing application folder (TEST-FIREFLY-DEPENDENCIES). This contains the PC GAMESS/Firefly Quantum Chemistry Package License Agreement (or else download it from the public PC-GAMESS/FIREFLY project website). If you do not agree with all the terms of this License Agreement, you cannot use the PC GAMESS and cannot apply for the installation key.

If you agree with the License Agreement, please read the "Registration_email_template.txt" document. Then, send the valid registration email to Dr. Alexander A. Granovsky (email: gran@classic.chem.msu.su) using "Registration_email_template.txt" as the template. Note that:

1. The subject field of your email must be "The PC GAMESS/Firefly registration".
2. Your email must be either plain text or html-formatted. **NO** attachments are allowed!
3. The only public e-mail service we accept emails from is Gmail. Otherwise, you **MUST** use your email account at your institution/organization.
4. The registration email **MUST** be written in English.
5. The header of your registration email (first 4 lines) **MUST** be exactly as in the Registration_email_template.txt.
6. You **MUST** answer questions #1 - #11, and exactly in the same order as specified.

The details of point 5 & 6 are shown below for your convenience (italicized for emphasis):

Dear Dr. Granovsky,

I agree with the terms of the PC GAMESS/Firefly Quantum Chemistry Package License Agreement. Please provide me the required installation key.

My registration information is summarized below as requested:

1. *Title (e.g., Mr., Ms., Dr., Prof., etc...)*
2. *Complete name (e.g., John C. Smith)*
3. *Position (e.g., student, graduated student, Engineer, Senior Researcher, Scientist, etc...)*
4. *Affiliation (e.g., Department of Chemistry, M.V. Lomonosov Moscow State University)*
5. *Postal address*
6. *Country (e.g., Russia, USA, Japan, etc...)*
7. *Contact email (e.g. alexey.a.popov@gmail.com)*
8. *Contact phone (including country and area codes)*
9. *The number of program copies you are planning to use (e.g., 1)*
10. *Operating System you plan to use (e.g., Leopard, Snow Leopard, etc...)*
11. *List of processor(s) you are planning to use to run program (e.g., Intel Core 2 Duo, Intel Xeon 5150 Quad, etc..)*
12. *Provide any additional comments or questions you may have*

Thank you in advance,

Your complete name (e.g., John C. Smith)

7. Registration emails which do not meet these requirements will not be considered.
 8. If you have problems filling in your registration email, see the "Registration_email_sample.txt" for a sample.
- If you still have any additional questions, contact Dr. Alexander A. Granovsky.

Your registration email will be answered within a couple of days. Upon receiving installation key, use it to run GAMESS/Firefly installer.

You **MUST** keep your installation key secure as it is the part of SOFTWARE and is subject to the same License Agreement as the PC GAMESS binaries themselves as stated in the License Agreement.

STAGE 3: Run the DMG installer

The newest official release will be posted on the PC-GAMESS/Firefly for Mac OS X webpage:

<http://classic.chem.msu.su/gran/gamess/macosex.html>

For the latest beta version use this link instead:

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

Thereafter, you should also visit the main project page for general news, updates, documentation and other things of interest such as the discussion forum (see links below).

<http://classic.chem.msu.su/gran/gamess/index.html>

Running the DMG installer is quite trivial as it mounts and install like any other Mac application. Please note that you **CANNOT** run this encrypted installer without the supplied license code that you will get by completing STAGE 2.

STAGE 4: Let's run some jobs

If you are so inclined, benchmarks tests are provided to ensure that you system is running normally and to compare your timing with other Mac users (this is useful to perform and more detailed instructions on running the benchmarks are contained in the complete install and usage guide). For the impatient or excited, we will proceed in this quick start usage guide directly onto instructions for how to run jobs.

I shall presume that you are familiar with how to create input files suitable to run on PC-GAMESS / Firefly and generally familiar with running with computational chemistry programs. If not, I would recommend pausing and reviewing the more complete installation and usage guide.

There are currently three ways to run PC-GAMESS / Firefly jobs on your Mac:

METHOD 1 (Graphical Drag and Drop Job Submission Run Applications)

There is a set of drag and drop run applications provided with your install package in the RUN-FIREFLY-JOBS directory. They can also be downloaded separately by using the URL download link below:

<http://classic.chem.msu.su/gran/gamess/macosx/RUN-FIREFLY-JOBS.zip>

A good idea, for example, it to copy the RUN-FIREFLY-JOBS folder to whatever location is most convenient for your computer and run your jobs from there. There are a total of six Mac job submission run applications, one GUI job termination application and one shell runscript contained in this download. The main seven native Mac applications located in the root of the “RUN-FIREFLY-JOBS” folder are:

Run-Firefly-Job-1-Core
Run-Firefly-Job-2-Cores
Run-Firefly-Job-4-Cores
Run-Firefly-Job-8-Cores
Run-Firefly-Job-Interactive
Run-Firefly-Job-Interactive-Batch
runpcgmac.sh
STOP-FIREFLY-JOBS

In addition, there are six specially configured Mac applications located in the “AUTO-OPEN-IN-GUI” subfolder of the main “RUN-FIREFLY-JOBS” folder and they are:

Run-Firefly-Job-1-Core-GUI
Run-Firefly-Job-Interactive-GUI
Run-Firefly-Job-2-Cores-GUI
Run-Firefly-Job-4-Cores-GUI
Run-Firefly-Job-8-Cores-GUI
Run-Firefly-Job-Interactive-Batch

A more complete discussion of each of the applications, their capabilities and limitations is detailed in this Stage 4, Method 1 portion of this documentation.

Single Job Submission Run Applications

(Everything except Run-Firefly-Job-Interactive-Batch)

The name of the applications pretty well explains their usage. Simply select and drag and drop your input file onto the run application and it will start your PC-GAMESS / Firefly jobs for you. In the case of the run applications that indicate the number of processor these programs will always submit your job with the number of processors in the name of the application. Any error messages or status information will be returned in the text window after the run application starts. If your job launches successfully, the output file will be written to the SAME directory as where the input file was located, with the .out extension added. The output file will be automatically opened with TextWrangler (one of the applications that has been installed to satisfy the dependency tests). As your job progress, the TextWrangler program will continuous display the current status of your output file. As the PC-GAMESS / Firefly programs continues your job, you will see the updated output results in real time in TextWrangler. In addition, a PUNCH file for your job will automatically be created in the same directory as the input file with the name INPUTFILENAME.DAT (just view your input file directory to see this).

If you wish to visualize this output file while a job is in progress (for example for a long geometry optimization), simply copy and paste this output file to an alternate location and open this copied file with a program of your choice (see below for suggested programs to visualize output files).

For the fifth application called “Run-Firefly-Interactive-Drop-Input-File-Here” this is a unified script that will allow you to select the number of processors that you wish to use after dragging and dropping your input file onto the run application.

Double-clicking all of these applications rather than dragging and dropping an input file onto them will prompt you to select an input file via a typical graphical interface (the final result is identical between dragging and dropping and double-clicking and then selecting a file).

Please note that all of these run application support concurrent job submission on the same script and from the same input directory (there are provisions to ensure that none of the temporary files and punch files will collide). For example, if you have four processing cores available, you could run the 1 processor script four times in succession or else when the 2 processor script twice in succession or lastly the 4 processor script one job at a time (You must wait for the previous job to terminate before starting another 4 processor job).

SPECIAL NOTES FOR Run-Firefly-Interactive-BATCH-Double-Click-Here Application

Use of this batch mode graphical job submission run application is very simple. Just double click on the application and a graphical interface will pop-up that asks you to select the number of processing cores that you wish to use for all input files that will be selected (current options are 1, 2, 4 or 8). Next a graphical interface

will pop-up that asks you to select the files that you wish to submit to this batch job application. There are no particular limits on the number of files selected but you may wish to keep it to something reasonable (perhaps 100 or less). Next, assuming that you have selected a valid number of cores for your machine and you have submitted valid input files, your jobs will begin to launch sequentially.

There are some notes regarding the differences between the other five single job submission run applications and this batch run application that you should be aware of.

- 1) You cannot drag and drop a set of files unto this batch job submission application. You must double click the application instead and select the files that you wish to run using this method. The other single job submission application supports both drag and drop and double click input methods.
- 2) The output file will NOT automatically open with TextWrangler soon after launching as it does with the single job submission run applications. TextWrangler will instead only launch after the job has COMPLETED.
- 3) Only ONE value for the number of processing cores is supported for all input files.
- 4) This batch run application does not optimize the resources on your computer, but rather just simply sequentially launches all of the input files supplied just as if launched from a command line. You will need to ensure manually that the number of processing cores selected and memory requested take full advantage of your resources.

These limitations may or may not be removed in future versions of the batch job submission run applications. As always you should report any bugs or features requests.

NOTE: This graphical batch job submission run application IS NOT suitable for running the benchmarks. Please use the benchmark runscripts as provided as some required options are not supported in the graphical batch runscript are that are needed for proper completion of these benchmark runs. Details on how to run the benchmarks as appropriate for your particular machine are contained in the complete install and usage guide.

SPECIAL NOTES ABOUT RUN APPLICATIONS IN THIS [AUTO-OPEN-IN-GUI](#) SUBFOLDER::

Run-Firefly-Job-1-Core-GUI

Run-Firefly-Job-Interactive-GUI

Run-Firefly-Job-2-Cores-GUI

Run-Firefly-Job-4-Cores-GUI

Run-Firefly-Job-8-Cores-GUI

Run-Firefly-Job-Interactive-Batch

These Firefly job submission run applications are identical to their counterparts in the main RUN-FIREFLY-JOBS folder except for the following two modifications:

1) All of these job launch applications will not close after the firefly job is started. This means that if you terminate these job launch applications, any Firefly job that was submitted by the application will also immediately terminate as well.

2) After submitting the Firefly job, each application will wait until the job is completed and then display the results in a text editor (TextWrangler is the result) and open the result of the job in a graphical visualization application (MacMolPlt is the default).

Please note that these job submission run applications will require that MacMolPlt is installed into the default location (the /Applications directory). You can download MacMolPlt if it is not already installed on your system by using the following URL below:

<http://www.scl.ameslab.gov/MacMolPlt/>

Please note that although MacMolPlt is the default graphical visualization application to open the completed job, this can be readily modified in the application internal .config file. The next section provides detailed information about how to modify the .config internal configuration files for ANY run applications.

HOW TO CUSTOMIZE YOUR GRAPHICAL JOB SUBMISSION/LAUNCH RUN APPLICATIONS

The default configuration options set for your job submission applications should (hopefully) prove quite suitable for the vast majority of Firefly for Mac users. There are, however, a number of customizations possible for all of the job submission run applications, mainly to support any non-default (non-standard) program installation paths and job launch options. This includes, but is not limited to, changing the number of processing cores to be used (for those applications that do not take this variable from a graphical dialog box), changing the absolute path of any dependency or helper application as well as the absolute path to the Firefly binary itself. In addition options such as custom scratch directory and file designations as well as opening the completed output file in a graphical visualization program can also be supported. If you are interested in making such changes to your Firefly for Mac job submission applications through modification of the internal configuration file, please read the complete install and usage notes (Mac_OS_X_PC-GAMESS-Firefly-Install_Notes_Usage_Guide.pdf) for the necessary instructions.

SPECIAL NOTES ON STOP-FIREFLY-JOBS application

The Mac application STOP-FIREFLY-JOBS must be double clicked to start (no drag and drop support for this application). Once started, the application will find all currently running Firefly for Mac jobs on your machine, provide a simple Yes-No pop-up dialog box with a short description of each Firefly job that is currently running and provide a prompt that allows you to terminate or not terminate each job found (Yes / No). In the text box that is automatically opened when the STOP-FIREFLY-JOBS application is started a more complete summary for each job is displayed and can be reviewed in greater detail if desired.

*****KNOWN LIMITATION FOR STOP-FIREFLY-JOBS APPLICATION!*****

For this application to work, you will need a 100% default installation of everything. This will mean that if you customized any of the application configuration (.config) files doing so may well break the STOP-FIREFLY-JOBS application. Due to limitations in the parsing code used for this application, if the absolute path to the input file used to run your Firefly for Mac job has any spaces in the any of the subdirectories or the actual input file name itself, this application will return nonsense data for the reported job parameters (or possibly no data at all). If this occurs, just answer “No” to the terminate job prompt for each job and correct the file path issue. There is currently no workaround for this issue. More generally, it is NOT a good idea to use spaces in directory names or file names when running on a UNIX system such as Mac OS X. While spaces in file names and directories is supported by OS X and most programs running on OS X, each instance of a filename or directory with a space or special character included requires a workaround to the ordinary UNIX conventions that do not support spaces. Thus the use of spaces in directory and file names needlessly increases the possibility of errors and crashes. It is recommended that any directories and filenames that are to be used in any way with the Firefly for Mac shall contain no spaces and no special characters. Good substitutes for spaces in filenames are the underscore “_” or dash “-“. As an example, my “input file 2 with spaces.inp” should become “input_file_2_with_spaces.inp” or else something like “input-file-2-with-spaces.inp”. Due to some limitations (truncation) in the ps UNIX utility under Tiger upon which this application relies, the STOP-FIREFLY-JOBS application is only supported for Leopard or newer versions of OS X.

Error Checking and Reality Check for your Job Runs

There is some rudimentary error checking in these run applications that will prevent you from running a single job submission on more cores than are present on your machine. If your job run request exceeds the number of cores on your machine, the run application will abort. You can, however, overrun the total number of cores available if you submit multiple jobs that in AGGREGATE exceed the total number of processing cores available. Be careful not to do this as it may make your system sluggish, unstable, or even crash. If this occurs, please refer to the complete install and usage guide as termination of PC-GAMESS / Firefly is covered in greater depth. In addition, care should be taken to not request more than the total PHYSICAL memory available on your machine as memory swapping could occur as a result giving very poor performance as a

result. It is encouraged to carefully monitor the progress and system usage of your job to ensure that everything is proceeding smoothly (the complete install and usage guide discusses the methods to check the real-time CPU and memory usage).

If you correctly choose your options, you can get efficiencies for many parallel jobs up to 99% for many direct SCF runs. Most single point energy type jobs should include the following two options for best parallel job run results:

```
$p2p p2p=.t. dlb=.t. $end
$scf dirscf=.t. $end
```

Most geometry optimization type jobs should include the use delocalized coordinates (DLCs) rather than Cartesian coordinates for best results. To enable this use `nzvar=1` (or other compatible `nzvar` setting) in `$contrl` group, and an extra card `$zmat dlc=.t. auto=.t. $end`. If Firefly fails to generate DLCs it probably means you have "disjointed" pieces in your molecule and you should add `nonvdw(1)=...` keyword to `$zmat` as appropriate to complete your zmatrix. Obviously choosing the DLC option means that your input coordinates must be in a zmatrix of one form or another. Please review the online documentation for further details as these two comments are only intended as suggestions for some of the most common optimizations.

Note: While conventional SCF jobs are fully supported with this PC-GAMESS / Firefly for Mac implementation, the file I/O limitations may limit the efficiency of such jobs.

METHOD 2 (Use the commandline `runpcgmac.sh` Runscript)

The `runpcgmac.sh` shell runscript is contained in the `RUN-FIREFLY-JOBS` directory (either downloaded separately or in the main distribution). The `runpcgmac.sh` shell runscript is an excellent way to run PC-GAMESS / Firefly jobs on your Macintosh if you are comfortable in the Terminal application and prefer running applications from a command line. For previous GAMESS-US for Mac users, this scrip will most resemble the `runrms` script that you have used in the past (please note that there significant differences however and you will need to read the usage instructions to get it to work correctly). **One of the most notable differences between the `runpcgmac.sh` script and the `runrms` script is that the path to the input file and output file parameters MUST BOTH BE ABSOLUTE to get a successful job run.** For example,

The following usages **WILL NOT** work:

```
./runpcgmac.sh inputfile1.inp outputfile1.out 2
```

```
./runpcgmac.sh ./inputfile1.inp ./outputfile1.out 2
```

But the following usage **WILL** work:

```
./runpcgmac.sh /Users/tpatko/Research/Firefly/inputfile1.inp /Users/tpatko/Research/Firefly/outputfile1.out 2
```

You can graphically drag and drop your input file onto the xterm Terminal application. This will return the absolute path of the input file that you drag and dropped onto the shell terminal (quite convenient).

As is usually the case, using the command line runscript version offers you the option to configure your runscript extensively. Detailed instructions on how to use this command line runscript are provided in the notes of the script itself. Simply open this shell script file with TextWrangler and read the usage notes carefully. Be careful not to modify the script unless you are certain of the changes that you are making as your changes may cause the script to not function normally. Most users will not need to make any changes to this runscript, but rather just read the usage instructions and submit the appropriate three parameters to run the script. The function of the graphical run applications and command line runscript is identical (the command line runscript also automatically open the resulting output file in TextWrangler, for example).

METHOD 3 (Pure command line execution string)

To run a PC-GAMESSS/FIREFLY job from a command line without any script or run application, just use the following guideline:

```
/Applications/Darwine/Wine.bundle/Contents/bin/wine /Applications/PC-GAMESS-FIREFLY-  
MAC/pcgameess.exe -osx ***
```

*** After the `-osx` switch followed by a space, please follow all of the normal PC-GAMESS/FIREFLY command line options as detailed in the enclosed in the readme folder. You can use the provided runscripts as a quick guideline for running some types of jobs. Consult the relevant manuals and the `runpcgmac.sh` commandline runscript for more complete information.

The paths selected for the input, output and scratch file locations are completely up to the user so long as you have read/write permission to that path. With this method, please note that ALL paths must be ABSOLUTE to get a successful job run. There are a couple of notes that can make it easier to use this job submission method:

- A) You can graphically drag and drop your input file onto the xterm Terminal application. This will return the absolute path of the input file that you drag and dropped onto the shell terminal (quite convenient).
- B) You can prepare your long execution string in a text editor such as TextWrangler using the benchmark runscripts as a guideline. Once ready, you can copy and paste this long execution string into your xterm terminal shell application and just run the job more conveniently.

If you wish to use this method to submit jobs, please review the benchmark runscripts in TextWrangler as a guideline as well as the standard documentation. In addition, if you wish to run submit batch job runs that require options not supported by the graphical batch job submission run application, then making an analogous

batch runscript to those shown in the benchmark runscripts is your best (and only) option. Running jobs using this method offers 100% control of the exact execution string, and 0% convenience in automating the process of job submission!

SPECIAL NOTES ABOUT RUNNING PC-GAMESS/FIREFLY UNDER WINE

Part 1:: Memory Limitations and OS Performance

Darwine is a fully open source implementation of the 32-bit Windows runtime environment (API). The maximum memory that can be allocated per process is 190MW (1520MB) under the current implementation. On an 8-core Mac Pro this means a maximum of 12160MB (~12GB+) total memory can be allocated for an 8-core parallel run job. For all other Mac machines with 2-cores total, this would mean that up to 3040MB (~3GB+) total memory can be allocated for a 2-core parallel job and 6080MB total memory can be allocated for a 4-core parallel job. **Users are encouraged to run all jobs as direct SCF calculations whenever possible (essentially sufficient memory is available), as there is some file I/O degradation running PC-GAMESS/FIREFLY under Wine that may result in slower runtime for non direct (conventional and semi-direct) SCF jobs.**

Appendix 1 :: Graphical User Interface (GUI) for Mac

Mac Native Applications to prepare input files and visualize output files

The following applications are tested and known to work on Mac OS X with PC-GAMESS/FIREFLY input and output files: WebMO (Both the Free and Commercial version), MacMolPlt, PCModel, Orbdraw and Vibrate (from Serenasoft). For WebMO, you will want to enable the PC-GAMESS/FIREFLY interface as the administrator and then prepare an input job as though you were planning to run it directly from WebMO (although you cannot actually do this at this time). Go to the Preview tab just before submitting the actual job. This will generate the text input for your job. Copy and paste this text into a text editor like TextWrangler and modify as appropriate to optimize your job run. Importing of PC-GAMESS/FIREFLY jobs run under Wine for Mac in WebMO proceeds just as it would if the PC-GAMESS / Firefly job was run under Linux or Windows.

<http://www.webmo.net/>

WebMO has specialized install instructions for Mac users (see below).

http://www.webmo.net/support/installation_osx.html

MacMolPlt (Free) and PCModel, Orbdraw & Vibrate (Commercial) can also prepare PC-GAMESS / Firefly compatible input files, and view (visualize) the resulting job output files (such as molecular orbitals, vibrational modes, spectra, ...etc). Please note that none of these programs can currently allow you to run a job directly from the GUI (not even WebMO). You should run your jobs using one of the three options described above.

<http://www.scl.ameslab.gov/~brett/MacMolPlt/>

<http://www.serenasoft.com/>

Marvin from ChemAxon (including MarvinSketch, MarvinView and MarvinSpace) is a very convenient and intuitive way to draw chemical structures in 2D or 3D. In particular it has an extensive fragment library and support custom fragment templates. Although Marvin does not allow you to prepare or visualize Firefly input and output files, the structures can then be exported via a variety of common file format (MDL .mol, Sybl .mol2, XYZ,) which can be imported into any of the programs described here to create the final Firefly input file. ChemAxon products are provided free of charge for academic users (registration required).

<http://www.chemaxon.com/products.html>

Windows Applications to prepare input files and visualize output files that have been successfully reported to run using some implementation of Wine or Windows Emulation

Gabedit (FREE)

<http://sites.google.com/site/allouchear/Home/gabedit>

Chemcraft (Commercial with Trial Version)

<http://www.chemcraftprog.com/>

Facio (FREE)

<http://www1.bbiiq.jp/zfffelis/Facio.html>

Crossover Wine for Mac (Commercial Implementation)

<http://www.codeweavers.com/products/cxmac/>

or Darwinie (Open Source Implementation)

<http://www.kronenberg.org/darwine/>

You will already have Darwinie installed as this is a strict dependency for running Firefly on your Mac.

If you have any difficulty running these programs under Crossover Wine or Darwinie you should definitely be able to run them with VMWare Fusion or Parallels.

<http://www.vmware.com/products/fusion/>

<http://www.parallels.com/>

Other software with successful results reading and visualizing PC-GAMESS input and output files on the Mac platform would be good to know.

PC-GAMESS / Firefly for Mac OS X Quick Start Install and Usage notes

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Last Revised February 16, 2009

PLEASE REFER TO THE COMPLETE INSTALL AND USAGE GUIDE FOR ADDITIONAL DETAILS SPECIFIC TO RUNNING FIREFLY ON MAC THA ARE NOT COVERED IN THE QUICK START GUIDE!

Corrections to this guide are encouraged, as are additions that would be mutually beneficial to future Mac users of the PC-GAMESS/FIREFLY QC program.