SHORT INTRODUCTION TO FIREFLY WITH EXPERIENCE IN HPC2015 AND HTC

SeyedAbdolreza Sadjadi and Darren ZhouRuiyi

HKU Laboratory for Space Research (LSR) and HKU Department of Chemistry ssadjadi@hku.hk & u3514033@connect.hku.hk

March 23, 2016

The 1st user special interest group (USIG) meeting on quantum chemistry , The university of Hong Kong

OUTLINES

- Brief introduction to firefly(PCGAMESS).
- Firefly on windows and linux operating systems
- Performance on HPC2015 and HTC systems.
- Abilities and Limitations.
- GABEIT a graphical Interface to firefly.

GENERAL ATOMIC AND MOLECULAR ELECTRONIC STRUCTURE SYSTEM (GAMESS)

- PCGAMESS (Firefly)
- Last version is : 8.1.1
- Running on windows, linux and mac (32 and 64 bit mode)

- Ab initio and Density Functional Theory calculations as well as simulation methods
- Free of Charge and can be downloaded:
- http://classic.chem.msu.su/gran/gamess/index.html

FIREFLY ON WINDOWS OS



Executable

FIREFLY COMMAND LINES ON WINDOWS OS

- D:
- cd D:\firefly8_windows\
- del oldpunch.dat
- rename punch oldpunch.dat
- SET INPUT=D:\firefly8_windows\H2O-RHF.inp
- Firefly8.exe -f >D:\firefly8_windows\H2O-RHF.out

FIREFLY COMMANDER (FICO) ON WINDOWS

plicat	tion	Tools	firefly811_windows					
Ma		FiCo -	Firefly Commander				-	- 🗆 🗡
	Inp	ut files a	nana			1		
		Setting	s		\times		Add Input File	Bun
		Firefly	Other					
		Firefly e	executable		CPU cores		Remove	Abort
) >		D:\firef	ly811_windows\Firefly811.exe		4		Edit as Text	Shutdown when done
~		Externa	l basis set library file (optional)					
		D:\firef	ly811_windows\Basis.lib				Edit geometry	
	Ou	Worki	ng directories					
		• AL	uto create		.out		Add Output File	
		D:\fir	efly811_windows		C _N.out		Remove	Settings
		C Lis	st		0 ?		View as Text	About
				Add				
				Remove			Show geometry	. Exit
	Ac			Kelliove				
								~
								<u> </u>
		Rem	nove temporary scratch files					
		Ford	es execution with old PUNCH or IRC	DATA files				
		Red	irects all text files to output file direct	tory				
	5	Addition	al command line options					
	Γ					2/3/2016	1:56 PM INP	File
	0					8/19/201	4 9:14 AM INP	File
	Γ		ОК С	ancel		10/25/20	14 10:59 LIB	File
v ·	c							

INPUT FILE FORMAT

The input file can be generated by any txt editors

\$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE \$END \$SYSTEM TIMLIM=60000 MEMORY=90000000 \$END \$BASIS GBASIS=N311 NGAUSS=6 NDFUNC=1 NPFUNC=1 **\$END** DIRSCF=.True. **\$END \$SCF \$GUESS GUESS=HUCKEL \$END \$DATA** Geometry optimization at RHF/6-311G(d,p) H2O **C**1 O 8.0 0.0 0.0 0.0 H 1.0 0.98 0.0 0.0 H 1.0 0.0 0.98 0.0 \$END

TESTING THE SOFTWARE

Run all the test input files in the sample folder

Bench 1

This is a RHF/6-31G* run on silacyclopropane, with 61 AOs.It comes from a study of cycloalkanes and silacycloalkanes by
J.A.Boatz, M.S.Gordon, and R.L.Hilderbrandt,
J.Am.Chem.Soc., 1988, 110, 352-358.

! The FINAL energy is -368.0867960698 after 10 iterations,! running the SCF in direct mode.

FIREFLY ON LINUX

Statically linked versionDynamically linked version

[~@hpc2015-file firefly811_mpich-1_ssh]\$ greetings.c greetings-pgiompi p4stuff.ex pbs-ff-simple.cmd pcgp2p.ex procgrp

FIREFLY COMMANDER (PBS) ON LINUX

#!/bin/sh

```
####PBS -I nodes=2:ppn=2
```

```
###export IMPI_HOME=/home/ssadjadi/mpich-install
###export PATH=$IMPI_HOME/bin:$PATH
###export LD_LIBRARY_PATH=$IMPI_HOME/lib:$LD_LIBRARY_PATH
export FFHOME=/home/ssadjadi/firefly811_mpich-1_ssh
export WORK_DIR=/home/ssadjadi/work
```

###export I_MPI_DEVICE="rdssm:OpenIB-cma"
###export I_MPI_DEBUG=10

cd \$WORK_DIR

time \$FFHOME/firefly811 -r -f -p -daf 2 -stdext -ex \$FFHOME -i \$FFHOME/Bench01.inp -o \$FFHOME/Bench01.out -p4pg \$FFHOME/procgrp -b \$FFHOME/Basis.lib

ABINITIO AND DFT CALCULATIONS

Geometry optimizations and Frequency calculations





B6C(2-) at B3LYP/6-311+G*

Foroutan-Nejad, C., Shafiee, G. H., Sadjadi, A., Shahbazian, S. Canadian Journal of Chemistry, Vol 84, Pages 771-781 (2006)

CALCULATIONS ON LARGE SYSTEMS C540 A nano size molecule



Semi-empirical (AM1) Geometry optimization and Frequency calculations

Within 359.8 min

On HTC platform

FIREFLY PERFORMANCE ON HTC PLATFORM

By using full CPU cores and threads

294.8 min was saved



FIREFLY PERFORMANCE ON HPC2015 PLATFORM

Firefly810 (MPICH-1), Second order perturbation theory, geometry optimization and harmonic frequency calculations. Cu2, MP2(FC)/aug-cc-pVTZ, 238 basis functions. Core electrons: 36, Correlated electrons: 22



PARALLEL VERSION (MPICH) RUNNING USING 3 PROCESSES (NODES)SMT aware parts of program will use2 threads.

The 1st user special interest group (USIG) meeting on quantum chemistry , The university of Hong Kong

SOME NOTES ABOUT FIREFLY

- Use exetyp=check in \$CONTRL to set the correct memory request and check if the jobs can be done on the hardware platform. This save much of your time for figuring out the correct memory/disk configurations and provide the efficient usage of computing resources.
- Memory can not exceed 260MW on Windows 64 bit
 \$SYSTEM MWORDS=250 \$END
- Semi-empirical calculations can not be done with more than 1012 atoms
- Coupled cluster (CC) calculations can be done by GAMESS(US). This version of GAMESS is available on HKU Gridpoint and it is very efficient coupled cluster code.

FIREFLY GRAPHICAL INTERFACE SOFTWARE

- Interface programs that help creating the input file and rendering/manupulating the information stored in the firefly output file
- Chemcraft
- Macmolplt
- Ghemical-GMS
- GABEDIT

GABEDIT THE FIREFLY INTERFACE WRITTEN BY: ABDUL-RAHMAN ALLOUCHE



BENCH 01

molecular structure



molecule formula: SiC2H6 charge:0 multiplicity:1 symmetry: C2v

The 1st user special interest group (USIG) meeting on quantum chemistry , The university of Hong Kong

TABLE OF BOND AND NON-BONDED DISTANCES

	distance	r(vdw)	r(covalent)	whether draw bond
r(Si-C)	1.8480995	3.19	1.88	yes
r(Si-H1)	1.4687996	2.79	1.43	no
r(Si-H2)	2.5643782	2.79	1.43	no
r(C-H1)	2.8745130	2.79	0.91	no
r(C-H2)	1.0767003	2.79	0.91	no
r(C-C)	1.5878680	3.4	1.36	no

FUNCTIONS PLOTTING IN GABEDIT

Molecular orbitals iso-surfaces

Electron location function (ELF)

Electron density iso-surfaces

The 1st user special interest group (USIG) meeting on quantum chemistry , The university of Hong Kong

ANIMATION OF VIBRATIONS IN GABEDIT

File Edit Insert View Geometry Tools Bun Settings Help	
Image: Construction Image: Construction<	
Recent Projects Data Result File Iools Help Gabedit : Orbitals/Density/Vibration Frequence Symmetry IR Int. Raman I 0.0400 Unknown 0.0000 0.0000 0.0000 0.0000 1 0.1800 Unknown 0.0000 0.0000 0.0000 3511. 3159. 2808. 2457. 2106. 1755. 1404. 1053. 702.2 351.1 0.1900 Unknown 0.0000 0.0000 0.0000 0.035 0.249 0.462	
Gabedit : Orbitals/Density/Vibration Frequence Symmetry IR Int. Raman I M 0.0400 Unknown 0.0000 0.0000 0.1800 Unknown 0.0000 0.0000 0.1900 Unknown 0.0000 0.0000 3.3300 Unknown 0.0003 0.0000 3.8100 Unknown 0.0010 0.0000 0.462 0.462 0.462	_
M 0.0400 Unknown 0.0000 0.0000 0.1800 Unknown 0.0000 0.0000 0.1900 Unknown 0.0000 0.0000 3.3300 Unknown 0.0000 0.0000 3.8100 Unknown 0.0000 0.0000 0.462 0.0402 0.462	
1 0.1800 Unknown 0.0000 0.0000 0.1800 Unknown 0.0000 0.0000 0.1900 Unknown 0.0000 0.0000 3.3300 Unknown 0.0003 0.0000 3.8100 Unknown 0.0010 0.0000	
0.1900 Unknown 0.0000 0.0000 3.3300 Unknown 0.0003 0.0000 3.8100 Unknown 0.0010 0.0000 - 0.462	0.000
3.3300 Unknown 0.0003 0.0000 3.8100 Unknown 0.0010 0.0000 - 0.462	-0.17
3.8100 Unknown 0.0010 0.0000 - 0.462	0.249
0.676-	0.462
5.7500 Unknown 0.0021 0.0000 0.889	0.889
Q 196.7900 Unknown 0.0110 0.0000 1.103	1.103
305.3700 Unknown 0.0254 0.0000	1.530
481.6100 Unknown 0.1732 0.0000 1.743	1.743
523.3000 Unknown 0.0059 0.0000 3511. 3159. 2808. 2457. 2106. 1755. 1404. 1053. 702.2 351.1	
574.5700 Unknown 0.0051 0.0000 cm ⁻¹	
779 3300 Unknown 0.2266 0.0000 X May: 2511 04 Half-Width : 20.000 Scale X : 1.000 Scale X : 1.	>cm-1
Mouse position: 3189.463/09, 2.333/74	
Scale factor : 0.500000	
Threshold(Bohr) : 0.001000	
Time step(s) : 0.100000	
Arrow radius : 0.100000	
Steps by cycle : 4	
Create a film BMP V Folder	
Play Stop	
File name : 1-3-cyclohexadiene-B3 File type : Dalton Geometry : Ok Mol. Orb. : N	
At. Orb. : Nothing	
Location Location Host : Abdi-Dell Host :	
Login :	
Directory :	9-51 AM
▲ ♀ □ Ҽ € <u>♥ ♥</u> <u>₽ ₽ ₽ ₩ <u>₽</u> <u>♥ ♥ <u>♥</u> ♥ ♥ ♥ ♥ <u>♥</u> <u>♥</u> ₽ ₽ ₽ ₽ ₽ ₽ ₽ ₽ ₽ ₽</u></u>	3/22/2016

JOB SUBMISSION AUTOMATION FOR FIREFLY ON HTC PLATFORM

Thank you Bill for helping us with this

ssadjadi@htclogin:~\$ ls 7z.dll exe firefly.bat README 7z.exe ff.7z firefly.con interlude.txt 7zip.dll ff800.7z gen_all.sh job.bat submit.condor ff811.7z.zip input

How to use

Put all your input files (*.inp) into the folder "input" Run chmod +x ./gen_all.sh Run ./gen_all.sh Run condor_submit submit.condor

CONCLUSIONS & REMARKS

- PCGAMESS over HTC and HPC2015 platfroms is reliable for Hartree-Fock, Post Hartree-Fock and Density Functional Theory calculations in combination with moderate and large size basis sets
- Moderate to large size molecules can be explored theoretically by present setup
- HTC is ready to cover the education and HPC 2015 for research purposes for broad range of users in different disciplines
- If a package of electron density analysis is installed on HTC and HPC2015 system, then the present computational chemistry services will reach to its ideal level.

We are grateful to our colleagues at ITS-High performance computing team:

Mr.Kwan, Miss Lillian Chan, Mr. Bill Yau and Dr. Mok Ngai Shing

Thank you for your attention