

Painless computational chemistry in the cloud with SCIGRESS

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■ Main objectives

- Aid everyday chemist's work
- **Reduce costs**
- Speed up research
- Limit environmental harm
- Make new discoveries
- Break less glassware ;)

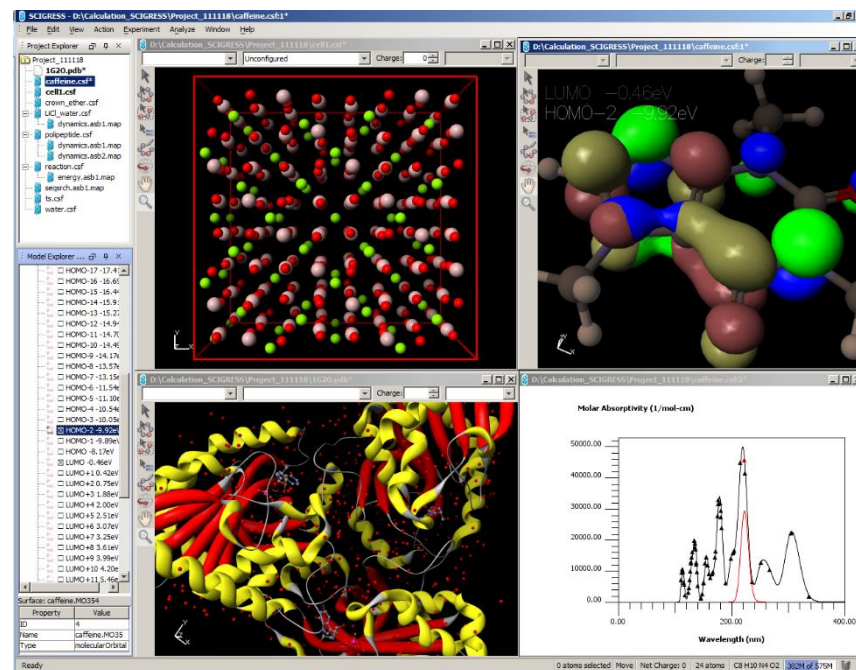
***"To the electron -- may it never be
of any use to anybody." -- JJ.***

Thomson's favorite toast



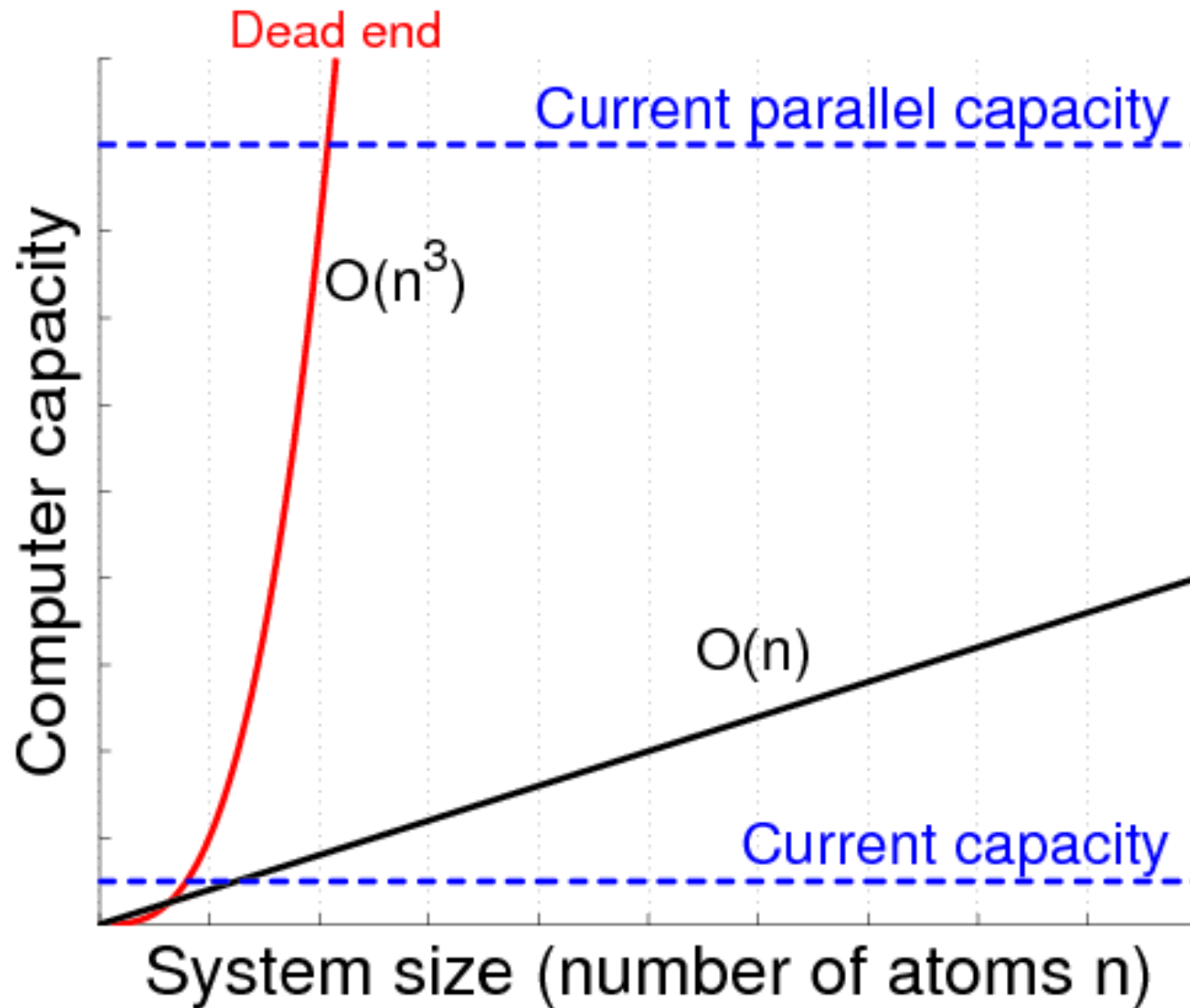
SCIGRESS at a glance

- Molecular Modeling & Molecular Dynamics Suite for Windows, Linux and Mac
- Fully integrated GUI, predefined computational procedures
- Builders for a range of systems
- Integrated engines MM to DFT
- Can run ADF, GAMESS, GAUSSIAN, LAMMPS, MOPAC 2012
- Quantum docking
- Batch calculations



<http://www.scigress.com> chemistry@fqs.pl

The problem



Solving basic needs by public providers



The cloud



Google Actual Cloud Platform, one of the company's April Fool's Day 2015 gags. [Google](#)

Where is the technological change?



No change *

* From user's perspective

Run remote calculations just as local ones

Computing resources

- 3,6+ PTFLOPS
- 90 000+ cores



Scientific Software

- 500+ applications, tools, libraries
- apps.plgrid.pl



Storage

- 20+ PB
- fast scratch
- distributed access



Tools for collaboration

- project tracking (JIRA)
- version control (Git)
- teleconferencing (Adobe Connect)



Computational Cloud

- PaaS based on OpenStack

- The PLGrid Infrastructure is available free of charge for Polish researchers and all those engaged in scientific activities in Poland
- On-line registration through PLGrid Users' Portal - portal.plgrid.pl
- User verification based on Polish Science Database - www.nauka-polska.pl



On PLGrid Users Portal user can

- apply for access to tools and services
- monitor utilization of resources
- manage their computational grants and grid certificates

Access to all PLGrid resources through **one account** and **one passphrase** (or grid certificate)



- Rimrock – Robust Remote Process and Job Controller
 - ease jobs submission and management on remote servers
 - submit.plgrid.pl
 - team:

- Daniel Haręźlak
- Marek Kasztelnik
- Maciej Pawlik



- PLG-Data team
 - easy access to data through web browser or other tools
 - data.plgrid.pl
 - team:

PLG-Data



The installation

- Minimal IT knowledge
- PLGrid credentials & Grant ID required
- Fully automated process
- **Nothing** to do for sysadmins

Upload SCIGRESS server

PLGrid generic

login: plgplonkaw host name: zeus.cyfronet.pl password:

grant ID: lgplonkaw2016b walltime: 2 h 0 min memory: 4096 MB submit queue: plgrid

SCIGRESS Server Deployable File

C:\plgrid\schedulerServerLin_04_05_2016.tar.bz2 Select

License

☒ online key: 6HRRG-PV32T-MNFU...HX

☐ file: Select

... operation in progress ...
... operation in progress ...
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0
Uploading license file
Copying PLGrid files
Setting grant ID in qsub script
Injecting walltime=02:00:00
Setting memory in qsub script
Switching MO-G to parallelized version
Upload sequence accomplished successfully

Upload Close

Choose what & where to compute

Run Procedure - ChemicalSample.csf

Input List
ChemicalSample: C:\Users\plonkaw\Documents\SCIGRESS\PLGrid_Test\ChemicalSample.csf
Set Inputs...

| Choose a category: | Choose a property: | Select a procedure: |
|--------------------------------|------------------------|-------------------------------------|
| chemical sample | optimized geometry | standard procedure |
| conformations | current energy | preoptimization (fastest) procedure |
| reaction and transition states | UV-visible transitions | MM (MM2) |
| excited states | IR transitions | MM (MM3) |
| docking | NMR spectra | MO-G AM1 |
| | | MO-G PM3 |
| | | MO-G PM5 |
| | | MO-G PM6 |
| | | MO-G RM1 |
| | | MO-G AM1 in water |
| | | MO-G PM3 in water |

Property and Procedure Description

optimized geometry: The structure of a chemical sample corresponding to an energy minimum

standard procedure: The structure of the chemical sample is refined by performing an optimize geometry calculation in MO-G using PM6 parameters.

[C:\Program Files\Fujitsu\SCIGRESS Suite\Procedure Library\Procedures.zip\OG_MO-G-PM6]

Edit... Delete

Server Info
plgrid://plgplonkaw@zeus.cyfronet.pl Select Server in 1 process

☐ Create a backup copy of the file before the procedure is run

Start Batch Cancel

Select Server

Available plug-ins:

- * FastDock - 1 process
- * ADFBAND - 4 processes
- * ADF - 4 processes
- * Phase - 1 process
- * CONFLEX - 1 process
- * Pubchem - 1 process
- * DGauss - 1 process
- * MO-S - 1 process
- * LocalSCF - 4 processes
- * Tabulator - 1 process
- * EHT - 1 process
- * LAMMPS - 4 processes
- * GAMESS - 4 processes
- * MD-ME - 1 process
- * Dynamics - 1 process
- * AmberTools - 1 process
- * MO-G - 4 processes
- * MOPAC2012 - 1 process
- * Mechanics - 1 process
- * Gaussian - 4 processes
- * ZINDO - 1 process

OK

Data transfer happens automagically

Procedure Status - ChemicalSample.csf (optimized geometry)

Stop... Retry Detach

Submitted: Thu, 1 Sep 2016 11:25:41

Started: Thu, 1 Sep 2016 11:26:05

State: Running

Server: plonkaw@wplonkaT1700@plgrid://plgplonkaw@zeus.cyfronet.pl

Input List

ChemicalSample: ChemicalSample.csf

☐ Close this window when done successfully

Calculating

DDI: 263624 bytes (0.3 MB / 0 MWords) used by master data server.

CPU timing information for all processes

=====

0: 56.871 + 6.559 = 63.430

1: 16.683 + 82.477 = 99.160

set exit_status=0

unset echo

----- accounting info -----

Files used on the master node n0686-g7x.zeus were:

-rw-r--r-- 1 plgplonkaw plgrid 1071 Sep 1 11:26 /scratch/67953336.batch.grid.cyf-kr.edu.pl/ChemicalSample.F05

-rw-r--r-- 1 plgplonkaw plgrid 100088896 Sep 1 11:28 /scratch/67953336.batch.grid.cyf-kr.edu.pl/ChemicalSample.F08

-rw-r--r-- 1 plgplonkaw plgrid 2355840 Sep 1 11:28 /scratch/67953336.batch.grid.cyf-kr.edu.pl/ChemicalSample.F10

-rw-r--r-- 1 plgplonkaw plgrid 794281 Sep 1 11:28 /scratch/67953336.batch.grid.cyf-kr.edu.pl/ChemicalSample.dat

-rw-r--r-- 1 plgplonkaw plgrid 15 Sep 1 11:26 /scratch/67953336.batch.grid.cyf-kr.edu.pl/ChemicalSample.nodes.mpd

ls: cannot access /scratch/67953336.batch.grid.cyf-kr.edu.pl/ChemicalSample-*.cube: No such file or directory

ls: cannot access /scratch/67953336.batch.grid.cyf-kr.edu.pl/ChemicalSample-*.grd: No such file or directory

ls: cannot access /scratch/67953336.batch.grid.cyf-kr.edu.pl/ChemicalSample-*.csv: No such file or directory

Thu Sep 1 11:28:58 CEST 2016

73.885u 89.439s 2:52.42 94.7% 0+0k 90864+2653648io 140pf+0w

Queue status: task is being calculated on 11:29:05

GAMESS finished successfully.

Calculations took 0h3m0s

Download Progress

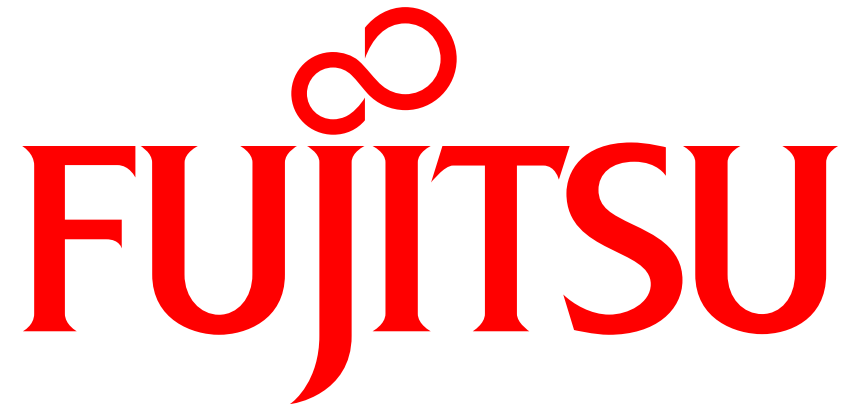
Downloaded 10MB

Cancel

Changes **may** come faster than expected



"Scientists from the RAND Corporation have created this model to illustrate how a home computer might look in the year 2004. However, the needed technology will not make it economically affordable for the average home. Also the scientists readily admit that the home computer will require not yet invented technology to actually work, but 50 years from now scientific progress is expected to have solved these problems. With teletype printer output and the Fortran language to program desired instructions, this computer will be easy to use."



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