Enabling Commercial Chemical Software on EGEE Grid – Gaussian VO

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EGEE'06, 26 September 2006

Outline

Computational Chemistry and Commercial Software

Why Commercial Software – do we need it?

YES!

- Most of the chemists use it in everyday's work
- New computational methods faster implemented
- Usually better user support
- More frequent bug fixes

Why Gaussian?

- One of the first *ab-initio* codes
- the most popular among chemical community
- variety of different QC methods implemented
- user-friendly

Gaussian VO

- Invented and operated by CYFRONET
- All license issues confirmed with Gaussian Inc,
- Open for every EGEE user
- Any computing center from EGEE with proper Gaussian license may support it
- VO manager – Mariusz Sterzel (m.sterzel@cyfronet.pl)

How to become a user?

Registration is open for every EGEE user

- Register at: https://voms.cyf-kr.edu.pl:8443/vo/gaussian/vomrs
- Accept Gaussian VO license requirements
- Wait for VOMRS admin acceptance
- voms-proxy-init --vo gaussian and you are ready to use the program...

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How to become a user?

- Accept Gaussian VO license requirements:
  1. I am not a member of a research group developing software competitive to Gaussian
  2. I will stop using Gaussian on EGEE Grid systems immediately and notify Gaussian VO manager (email: m.sterzel@cyfronet.pl) if there is a change in my situation that would bring into a question my status with respect to point 1 above
  3. I will not copy the Gaussian software, nor make it available to anyone else
  4. I will acknowledge Gaussian Inc, in published works to which Gaussian calculations on the EGEE Grid systems contributed

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Possible user problems...

Gaussian checkpoint file

- almost ever needed by user
- binary file...
- very often used in subsequent calculations or for restarts

Grid Solution:

- file should be always created
- user receives/sends only formatted version of it
- before computation starts binary version has to be recreated
- a script doing this is available at www.egee-grid.cyfronet.pl/Applications/Useful Scripts

How to support Gaussian VO

Computing centers with **Gaussian site license**

- e-mail to VO manager (m.sterzel@cyfronet.pl) concerning participation with site name and address
- VO manager confirms the site license status with Gaussian Inc,
- installation instructions at www.egee-grid.cyfronet.pl/Applications/Gaussian VO – how to support

Centers without **site Gaussian license**

- Must buy additional license from Gaussian Inc, NO EXEPTIONS!

Sample calculations – Vibrational averaging

Which effect we recover?

- Every QC calculations determine **electronic** structure of a molecule only
- From harmonic oscillator – nuclei never stop even at 0 K
- Vibrational average tries to give answer what is the effect of moving nuclei on a given molecular property

Numerical procedure

- vibrational frequencies
- calculation of molecular property at "slightly" displaced geometry along each normal mode
- $$-\frac{1}{4}\sum_{i}^{m}\frac{1}{\omega_i^2\sqrt{\mu_i}}\frac{\partial P}{\partial Q_i}\sum_{j}^{m}\frac{k_{ijj}}{\omega_j\,\mu_j\sqrt{\mu_i}}+\frac{1}{4}\sum_{i}^{m}\frac{1}{\omega_i\mu_i}\frac{\partial^2 P}{\partial Q_i^2}$$

^{195}Pt NMR chemical shifts of $PtCl_4^{2-}$ with resp. $PtCl_6^{2-}$

Computational details

- Method B3LYP with TZVP//QZVP quality all electron basis set
- $2 \cdot (3 \cdot N - 6) + 1$ single point NMR calculations done for each molecule
- all calculations done in water (default g03 conductor-like model)

Result:

^{195}Pt NMR chemical shifts of $PtCl_4^{2-}$	–1528 ppm
^{195}Pt NMR chemical shifts of $PtCl_4^{2-}$ with ZPVC	–1628 ppm
Experimental value:	–1630 ppm

Acknowledgment

We wish to thank Gaussian Inc, for help during work on license issues. M.S. wishes to thank Brendan C. Mort for allowing use of his ZPVC program.