WAVEFUNCTION

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I'd like to share with you the features under development for the release of ***Spartan'14***, later this year.

Spartan'14 ("***Spartan***") is designed to address the ever increasing role that calculations play in chemistry and related fields. It represents a continued collaboration between Wavefunction, Inc., and Q-Chem, Inc. Q-Chem codes supplement and extend the traditional strengths of ***Spartan*** as an easy to learn and use tool for molecular mechanics, semi-empirical and Hartree-Fock molecular orbital calculations, as well as a wide variety of graphical models, with a full range of density functional models and a selection of wavefunction based important post-Hartree-Fock models. All models have been implemented using what we believe are the most robust algorithms currently available, and have been tuned for high performance on Intel and AMD processors including multi-core processors.

Spartan'14 will support under Windows (Vista, 7, and 8, 32 and 64-bit), Macintosh (OS 10.6, 10.7, and 10.8), Linux (Linux Kernel 2.6 or later). The Linux version may also be used in a server mode with another Spartan for Windows or Linux license acting as a front end.

Features under development for ***Spartan'14*** include the following:

Building

Borrowing from development efforts on the iPad, we plan to include a 2D sketch builder for Spartan'14, providing for the easy constructions of molecules based on 2D rings, groups, and elements. The link between Spartan and ChemDraw (Windows only) will also be available for constructing in 2D for Windows user's that have licenses of both applications.

Spectroscopy

Improved Scoring for IR Spectral Matching A new scheme consistently provides excellent matches of calculated and experimental spectra (where the structure is known), allowing description of the motions responsible for the different lines in an experimental spectrum. It is much more successful than the previous implementation in ***Spartan'10*** for assigning structure based on the infrared spectrum.

NIST IR Database Search This provides the ability to match an infrared spectrum with an entry in the NIST experimental infrared database.

Improved Proton NMR Chemical Shifts This is an extension of previous work done with ^{13}C NMR spectra. Current RMS error is around 0.2 ppm, representing a vast improvement. We are quite confident in the performance of both proton and ^{13}C chemical shift predictions from calculation.

Improved Proton NMR Coupling Constants The previous empirical procedure for estimating proton-proton coupling constants has been completely revamped and performs quite well.

Plots

In addition to implementing Ramachandran Plots[1] for files brought in from the PDB[2]. The plot capability released in ***Spartan Student version 5*** will be carried forward to ***Spartan'14*** and will be extended to 2D NMR plots. This is a significant improvement over what exists in ***Spartan'10*** (and will be noticed by most users as such). The older Open GL based plotting will remain available for backward compatibility and legacy purposes.

The availability of 2D sketches and plots will allow users to easily paste into a Word or PowerPoint document.

Databases

Spartan Spectra & Propertied Database (SSPD) This will comprise ~250,000 molecules at the time of Spartan'14's release, including ~2,000 organometallic systems. The data model is moving to encompass the InChi format(away from SMILES). This allows ions and radicals to be easily stored. The SSPD will contain several thousand protonated and deprotonated forms (for the neutral acids and bases presently available in SSPD), and acidity and basicity will be accessible as properties. InChi also allows for automatic identification and substitution of tautomers.

Data Mining Extensions Data mining allows access to all information relating to molecular structure, properties and spectra contained in SMD and SSPD (presently >600K entries in total). The primary objective is to allow relationships among different quantities or combinations of quantities to be examined across entire series of molecules. Information retrieved from mining may be presented in the form of histograms or XY plots and may be used as the basis for linear regression. Data mining opens up a wealth of information to exploration. A means for introducing experimental data into the database dialog will be provided.

Parallel Computation

Vibrational frequency calculation has been parallelized for Hartree-Fock and density functional models, resulting in a speed improvement of approximately 1.8 for a two-core machine and 3.2 for a four-core machine. RIMP2[3,4,5] has also been parallelized, along with the T1[6] procedure. Additional components to be parallelized include graphical surface/map generation and IR spectral search. Parallel implementation of the NMR code is also under investigation.

Infrastructure

Tabs. Each open molecule is now given a "tab", any or all of which may either be turned "on" of "off". All tabs "on" mimics ***Spartan's*** previous display paradigm (all open molecules are displayed). Turning tabs "off" simplifies screen clutter.

File Compression. Files generated from ***Spartan*** (.spartan files) have been significantly reduced in size due to elimination of the part of the wavefunction that is not used, to file compression and (optionally) reduction of precision. This reduction ranges from a factor of five to between one and two orders of magnitude.

Monitor. The ***Spartan*** job monitor has been extended to allow "real-time" visualization of molecular structure. This means that progress of a geometry/transition-state geometry optimization can be followed.

Documentation

User's Guide & Tutorials Are accessible in PDF format from the Help Menu with the latter also available as individual PDF files (one per tutorial) from the Activities Menu. The Activities Menu also includes a series of Topic based entries spanning a wide range of computational topics.

Wavefunction, Inc.
www.wavefun.com
sales@wavefun.com

References:

1 Ramachandran G. N., Ramakrishan C., Sasisekharan V. (July 1963). "Stereochemistry of polypeptide chain configurations". *J. Mol. Biol.* **7**: 95–9. PMID 13990617

2 Protein Data Bank (www.pdb.org). H.M.Berman, J. Westbrook, Z. Feng, T.N. Bhat, H. Weissig, I.N. Shindyalov, P.E. Bourne (2000) "The Protein Data Bank". *Nucleic Acids Research* (Oxford Journals) **28:** 235-242.

3 Martin Feyereisena, George Fitzgeralda and Andrew Komornickib (May 10, 1993). "Scaled Second-Order Perturbation Corrections to Configuration Interaction Singles: Efficient and Reliable Excitation Energy Methods". *Chemical Physics Letters* (Elsevier) **208 (5-6)**: 359-363. doi:10.1016/0009-2614(93)87156-W.

4 Florian Weigend and Marco Häser (October 13, 1997). "RI-MP2: first derivatives and global consistency". *Theoretical Chemistry Accounts* (Springer Berlin / Heidelberg) **97 (1-4)**: 331-340. doi:10.1007/s002140050269.

5 Robert A. Distasio JR., Ryan P. Steele, Young Min Rhee, Yihan Shao, and Martin Head-Gordon (April 15, 2007). "An improved algorithm for analytical gradient evaluation in resolution-of-the-identity second-order Møller-Plesset perturbation theory: Application to alanine tetrapeptide conformational analysis". *Journal of Computational Chemistry* (Wiley InterScience) **28 (5)**: 839-856. doi:10.1002/jcc.20604

6 William S. Ohlinger, Philip E. Klunzinger, Bernard J. Deppmeier, and Warren J. Hehre (January 2009). "Efficient Calculation of Heats of Formation". *The Journal of Physical Chemistry A* (ACS Publications) **113 (10)**: 2165-2175. doi:10.1021/jp810144q