

LocalSCF

2003

Quantum Breakthrough in QM Modeling of Ultra Large Protein Systems

For the first time quantum-chemistry calculations of large (100,000+ atoms) real-life complex 3D proteins has been made available on a personal computer:

- ✓ Quantum-mechanics level of theory for protein modeling.
- ✓ Very fast calculations.
- ✓ Small resource requirement.
- ✓ Complex real-life protein systems.

Advanced geometry optimization options:

- Recognition of protein structure from Cartesian coordinates.
- Structured quality checking and verification.
- Identification of various molecular fragments: amino acid backbone, side-chain, terminal atoms, water molecules, and counterions.
- Intuitive and easy to use interface for specification of geometry optimization modes by defining particular fragments or amino acid numbers.
- Keyword based recognition and on-fly optimization of drug molecules in the enzyme cavity.

Linear scaling solvation model:

- Continuum conductor like screening model implemented.
- Small additional resource requirement with multiplier 2 for memory versus the gas phase mode.
- Geometry optimization in COSMO model.

Fast Multipole Method:

- Assures very low memory requirement, extremely fast calculation of large systems and high accuracy of evaluation of Coulomb interactions.
- Provides flexible control over the resource consumption.

True variational linear scaling method:

- Retains high accuracy for short localized molecular orbitals (the shorter LMOs the less RAM is consumed).
- Provides an optimal user-controllable balance between speed and accuracy.
- The built-in mechanism for accuracy validation allows comparison of molecular properties in connection with particular keyword options.

Program capabilities:

- Runs on popular PC platform.
- Ultra large 100,000+ atoms' protein systems.
- Very fast advanced geometry optimization specially tuned for proteins.
- Powerful control options for balancing between speed and accuracy.
- Linear scaling COSMO solvation model.
- Fast Multipole Method for evaluation of Coulomb integrals.
- True variational linear scalability.
- Semi-empirical Hamiltonians: MNDO, AM1, PM3, and PM5.
- File interface to CAChe and BioAdviser graphical user interfaces.
- One month free evaluation of full functional program.

Computer platform:

Pentium ® compatible personal computer

Microsoft ® Windows2000 or WindowsXP operating system

Ultra large systems:

Hsluv protease-chaperone complex (PDB 1G3I)

Number of atoms: 91,509

RAM: 1 Gb

Energy calculation: 6 hours on Pentium-4 @ 2.4GHz desktop computer

Precision mode: High Accuracy in semi-empirical partial atomic charges (RMS error = 0.001)

Fast geometry optimization:

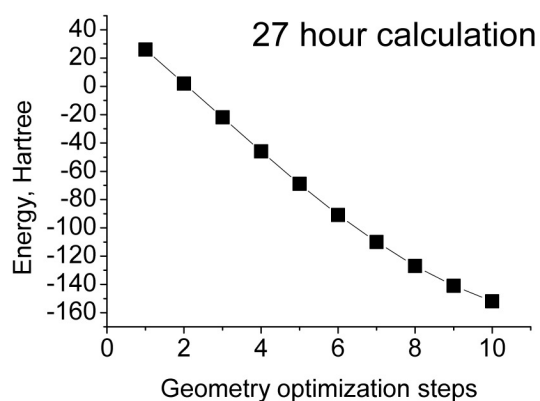
Energy convergence in full geometry optimization of 1G3I

Number of atoms: 91,509

RAM: 900 Mb

Full geometry optimization: 10 steps for 27 hours

Precision mode: Ultra Fast



Reference:

N.A. Anikin, V.M. Anisimov, V.L. Bugaenko, V.V Bobrikov, A.M. Andreyev, Chem.Phys. Letters, 2003 (in press). On-line preprint: <http://preprint.chemweb.com/physchem/0304005>

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