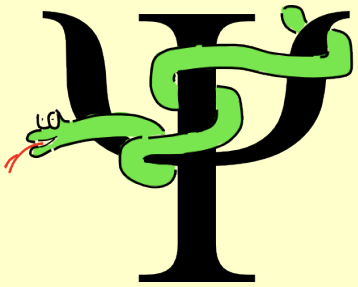
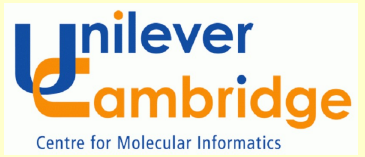


cclib

Parsers and algorithms for computational chemists



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Overview of cclib

- cclib is a programming library which
  - contains parsers for output files of computational chemistry codes
  - includes several algorithms for analysing results
- cclib is written in Python
- cclib is Open Source (LGPL)

Why is cclib needed?

- Analysis methods are available only to users of certain packages
  - Morokuma energy decomposition (implemented in GAMESS)
  - Charge Decomposition Analysis (Frenking's code only reads Gaussian output files)
- Keeps up to date with new versions of packages
- Allows chemists to focus on algorithms
- Makes implementation of algorithms independent of proprietary software

Parsers

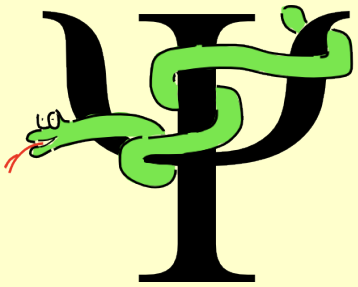
- ADF, GAMESS (US), Gaussian, PC GAMESS (GAMESS-UK, Jaguar, Molpro)
- Useful information for algorithms
  - overlap matrix, molecular orbital coefficients, (basis set coefficients, Hessian)
- Useful information for visualisation
  - coordinates, vibrational frequencies, electronic transitions
- Currently used by GaussSum and PyMOlyze

Algorithms

- Population analysis algorithms
  - Mulliken, C^2, Mayer's bond orders
- We are currently working on
  - Calculation of the electron density
  - Calculation of the Cartesian displacement matrix
- We intend to implement
  - Bader's Atoms in Molecules
  - Frenking's Charge Decomposition Analysis
  - Hirshfeld Population Analysis

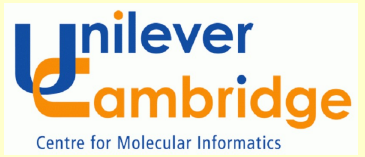
Development

- Follows Open Source development model
  - Subversion, wiki, mailing lists, bug tracker
- Follows best practice for Python
  - Cheesecake index, pylint
- Extensive use of unit tests and regression tests (test-driven development)
  - Parsers developed on example log files and the result must agree with the other parsers
  - Modified to cope with real-life problem cases



cclib

Parsers and algorithms for computational chemists



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Thank you...
...and new developers welcome!

http://cclib.sf.net **baoilleach@gmail.com**