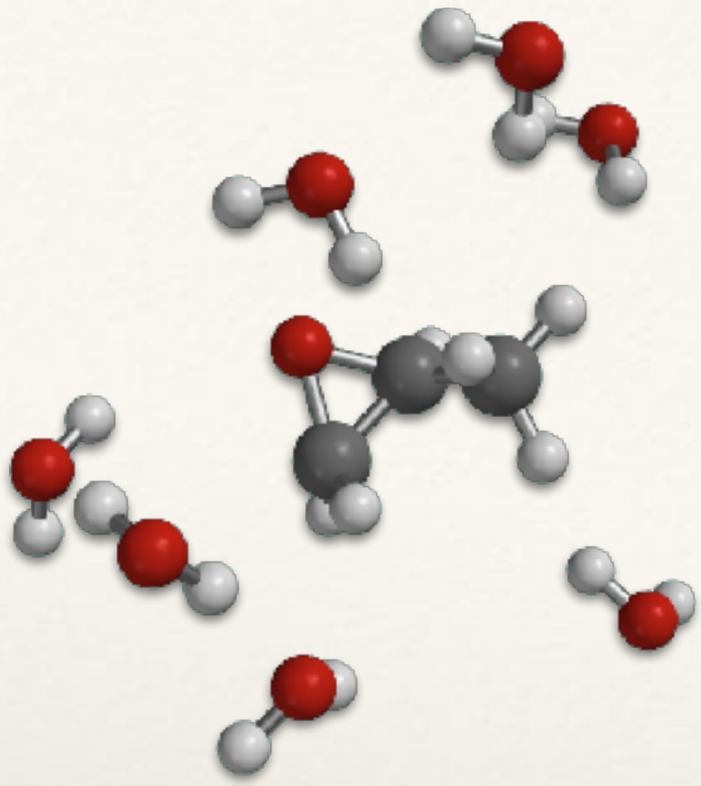

An Alternative N-body plugin

Properties

BSSE

(and Gaussian integration)

Ben Peyton
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github.com/bgpeyton/n_body

Psi4 Developers Conference 2017

What do I want?

- Chiroptical properties of small molecules in solution
  - Parallelized many-body expansion to cover cost
  - BSSE corrections to cover convergence issues[1,2]
    - SSFC, VMFC, hybrid schemes . . .
  - New n-body plugin required

[1] Mach, T. J.; Crawford, T. D. *Theor. Chem. Acc.* 2014, *133*, 1–9

[2] Skwara, B.; Bartkowiak, W.; Da Silva, D. L. *Theor. Chem. Acc.* 2009, *122*, 127–136

What is new?

- Properties
- Basic parallelization
  - Separate input file generation / “sowing”
  - Individual job submission
  - Proper storage / “reaping” of data
- Gaussian integration
  - For properties not available in Psi4 (TD-DFT)

What needs to be done?

- *Sow*
  - Generate input files (BSSE? Gaussian?)
- *Submit*
  - Current focus on VT ARC clusters
- *Reap*
  - Currently parsing output files (I walk through the valley of the shadow of death…)

. . . I need the Common Driver! (And TD-DFT)