Molecular density functional theory under homogenous reference fluid approximation

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- This thesis should contain a complete study of MDFT ender HRF approximation.

Theory

- All the frontier research domains of solvation properties prediction and liquid simulation (MDFT, IET, DFT, DM, Poisson-Boltzmann, etc.): models and methods.
- The main principle of MDFT (HRF) and MOZ (bulk properties), as well as its advantage / shortage compared to other methods.
- The output solvation properties: free energy, structure, basic state functions (thermodynamics quantities), etc.
- The limits of previous studies, and the capability of the present work (theoretically).

Implementation

- The main structure of code MDFT.
- Optimization: systematic comparison of computing efficiency (timing), brief discussion between memory limited and performance limited modes.
- Parallelization of node-level: OpenMP.
- Parallelization several nodes: MPI.
- Visualization of outputs: MDFT Viewer.

Validation

- Comparison with molecular integral equations theory, molecular dynamics and experiments: LJ centers, ions, and molecules. "Chemical accuracy" and "efficiency".
- Limits (energy accuracy, structure deformation, basic state functions) of method, advantages compared to reference methods and previous work.

Application

- Bank of 500 molecules.
- Hydrogen transfer reaction of Mn-oxo in DMSO: role of solvent in reaction simulation.
- Calculation of proton-coupled electron transfer mechanism by (Gaussian and) MDFT.

Perspective

- Possible new methods and algorithms to surpass actual limits.
- Application domains.