Optimizing 3D Structure of H_2O Molecule Using DDPG

Joanne Taery Kim[1,2], Soo Kyung Kim[1], Peggy Li[1], Piyush Karande[1], T. Yong Han[1]

Lawrence Livermore National Laboratory[1], Korea University[2]

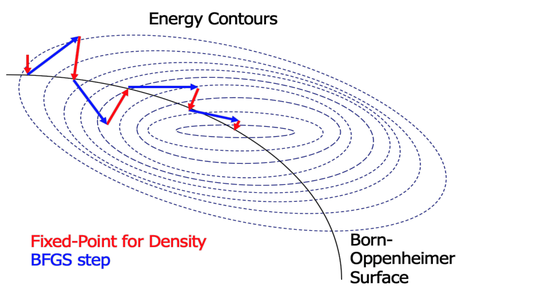
Abstract

- Conventional methods to predict 3D structure of molecule are based on iterative stochastic optimization techniques based on energy calculation using physics-based electronic structure modeling such as DFT or MD.
- Therefore, computing cost of physics-based modeling is significantly depended by the number of iterations to calculate energy until the total energy of structure is converged.
- As the cost-efficient alternatives, we propose a novel RL-based algorithm to optimize 3D structure of single H_2O molecule based on DDPG (Deep Deterministic Policy Gradient) method.
- To demonstrate the efficiency of our model, we predicted 3D structure of H_2O molecule and compared with results from the conventional DFT calculation.
- Our experiments show that our model succeed to predict 3D structure of H_2O molecule which is identical with the results from DFT calculation.

Molecular geometry optimization

Conventional Method

- Optimization algorithm can use some or all of $\boldsymbol{E(r)}$, $\frac{\delta E}{\delta r}$, and $\frac{\delta\delta E}{\delta r_i \delta r_j}$
- **Minimize the forces and energy**
- Example: gradient descent, conjugate gradient, or Newton's method.

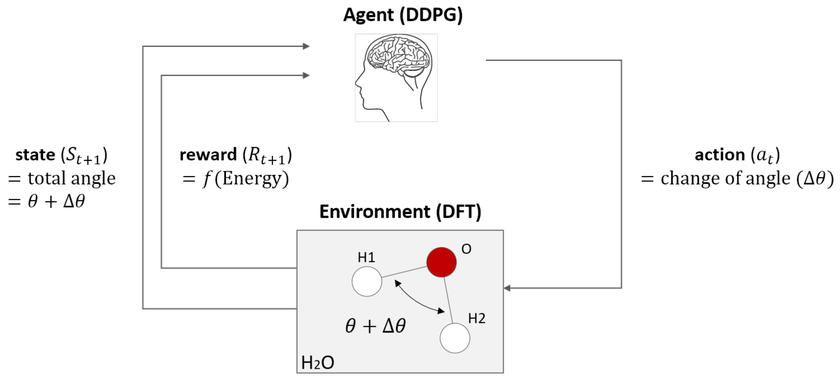


J. Chem. Theory Comput., DOI: 10.1021/ct4001685

Problem and Motivation

- Can find local minimum but difficult to find the ***global minimum***
  → **Exploration of RL** technique make structure **hop between potential energy surface**
- After training, **agent know fastest trajectory to global minimum**

Proposed Model



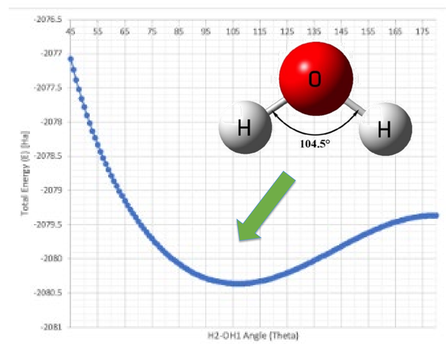
$O-H1$ bond length	0.96 Å
$H2-OH1$ bond angle	θ
Energy	E
Molecular structure generator	$\boldsymbol{m}$
Energy calculator (DFT)	$\boldsymbol{g}$
Reward function	$\boldsymbol{f}$

1. Initial molecule starts from random angle between 45° to 180°
2. Each iteration, agent changes angle and $\boldsymbol{m}$ updates 3D structure
   → DFT ($\boldsymbol{g}$) calculate energy from updated 3D structure
   $$\text{updated-geometry} = \boldsymbol{m}(\theta)$$
   $$E = \boldsymbol{g}(\boldsymbol{m}(\theta))$$
3. Reward $\boldsymbol{f}$ is computed accordingly

- Environment (g): Use Fhi-aims software (DFT)
- Modified OpenAI Gym setting

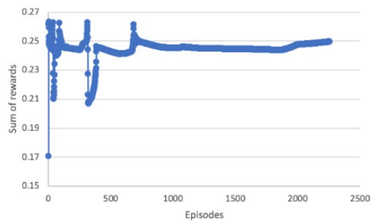
- **State (s_t):**
  Current angle and Current computed total energy
  $$\{\theta, E\}, \text{where } \theta_t = \theta_{t-1} + \Delta\theta$$
  $$\theta \in \{-45°, 180°\}, E \in \{0°, 1°\}$$
- **Action (a_t):**
  Change of angle
  $$\{\Delta\theta\}, \text{where } \Delta\theta \in \{-45°, 45°\}$$
- **Reward (r_t):**
  Weighted sum of decrease of total energy compared with previous step and decrease of total energy compared with the lowest energy founded so far.
  $$\text{Lowest-energy} = E_{low}$$
  $$\text{Current-energy} = E_i$$
  $$\text{Previous-energy} = E_{i-1}$$
  $$\boldsymbol{f}(E_{low}, E_i, E_{i-1}) = \alpha(E_{i-1} - E_i) + \beta(E_{low} - E_i)$$

Results

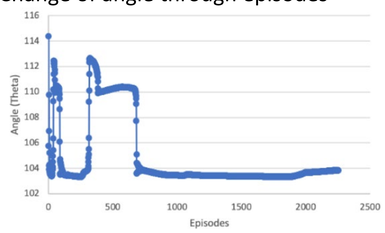


▲Potential Energy Surface of H_2O molecule of DFT energy by changing H2-OH1 angle

- Cumulative reward through episodes



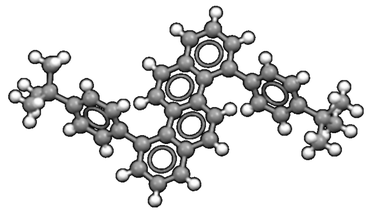
- Change of angle through episodes



After ~2300 episode the agent finds answer in few steps.

Future works

◆Optimizing 3D structure of aromatic hydrocarbon molecules



- Aromatic hydrocarbon family:
  - Only H and C atom
  - Repeated ring structure, simple and similar
- **Learn physics using RL**
  Transfer policy learned from several aromatic hydrocarbon molecules to new molecule yet to be analyzed.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

LLNL-POST-777137