MD and Reactions

Eric Hartmann

2023-10-02
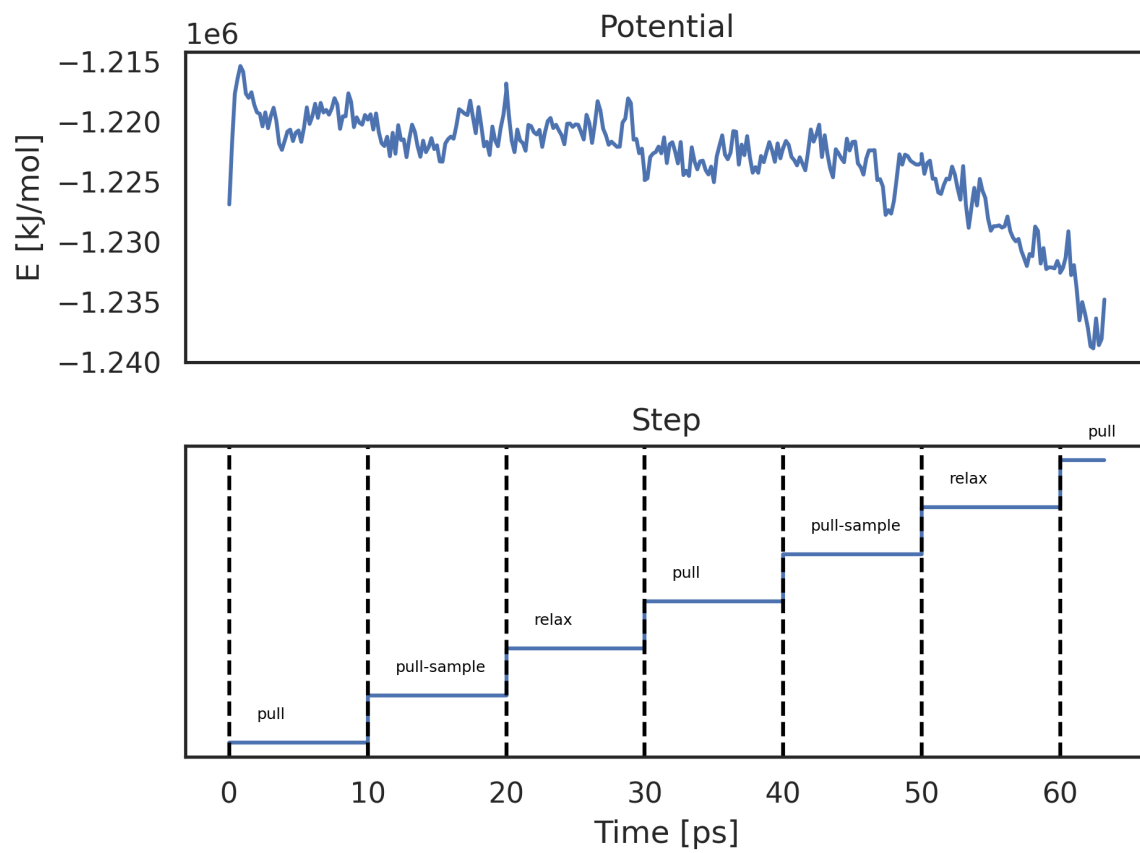
KIMMDY structure and theory

Practice

KIMMDY can break a tripelhelix (and continue simulating for a bit)
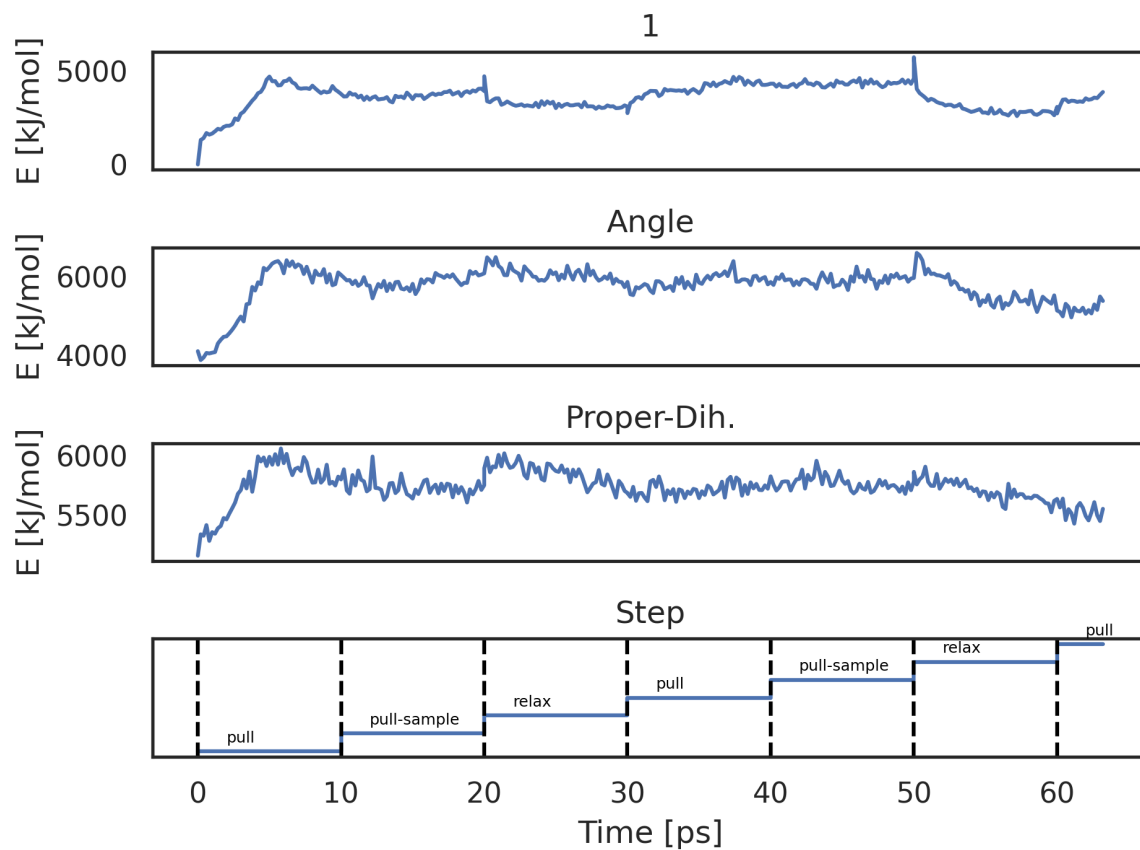
System energy is continuous

```
kimmdy-analysis energy <run_dir> -t Potential
```
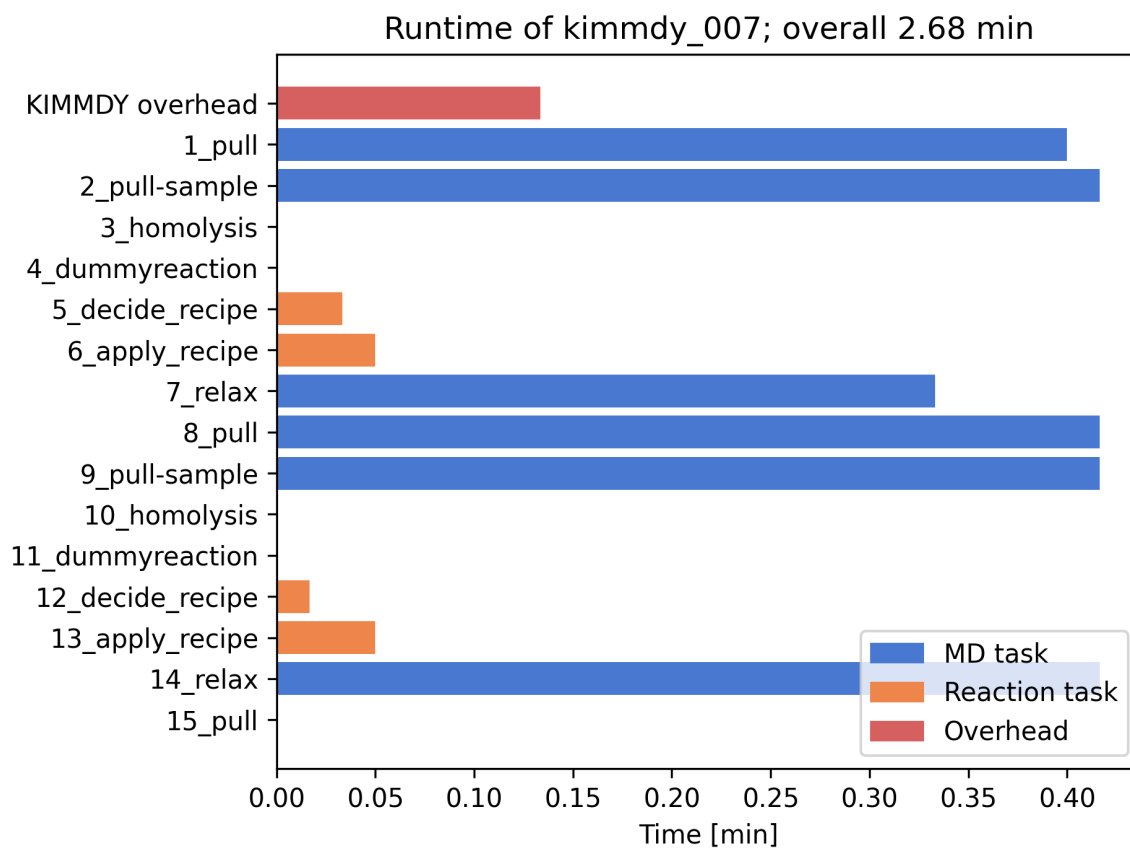
Intramolecular energy is continuous

```
kimmdy-analysis energy <run_dir> -t 1 Angle Proper-Dih.
```
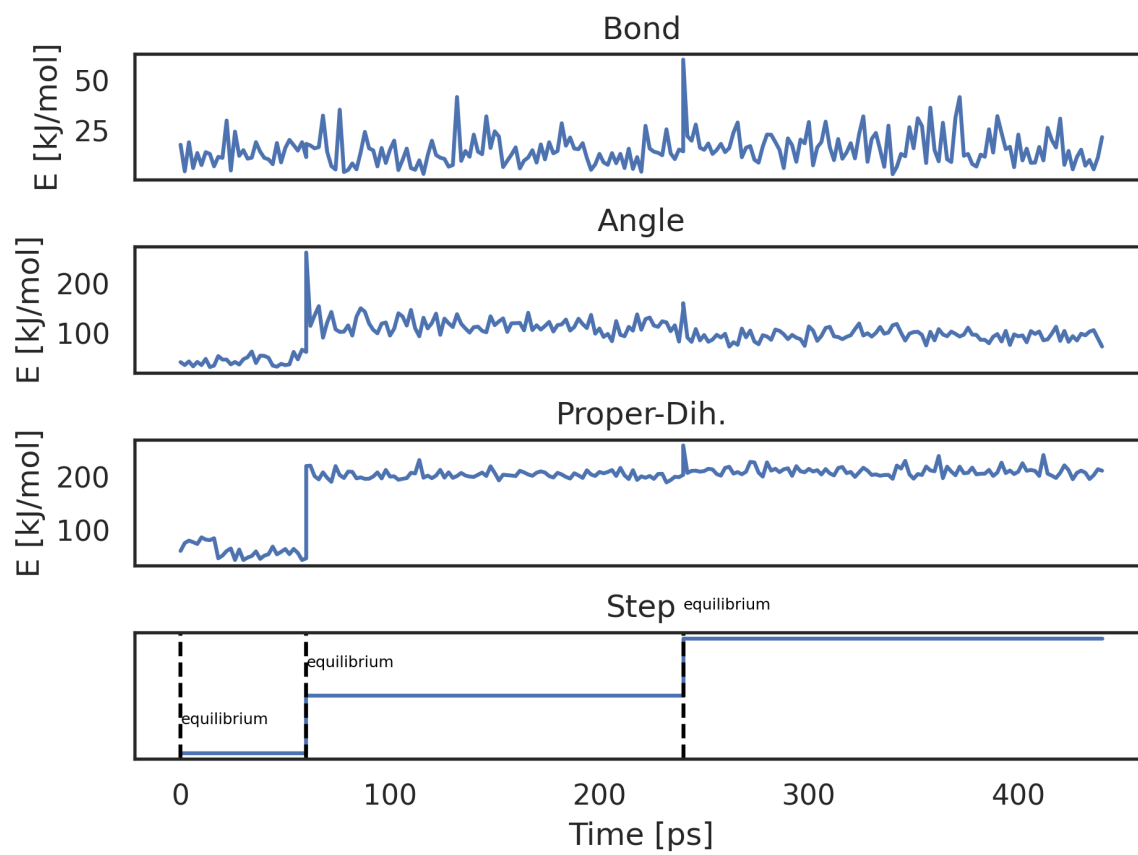
Most of the time is spend on MD

```
kimmdy-analysis runtime <run_dir>
```

Runtime of kimmdy_007; overall 2.68 min

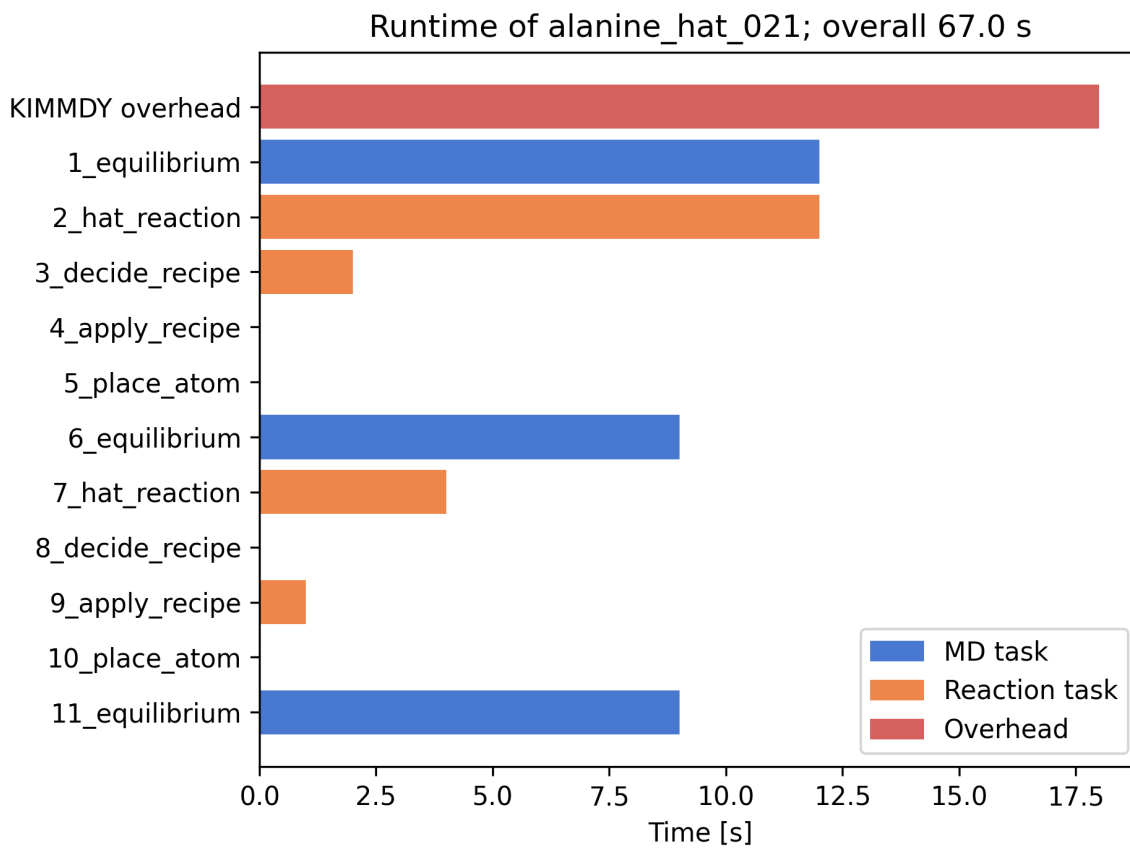**KIMMDY can simulate HATs**

Intramolecular energy behaves almost physically correct

```
kimmdy-analysis energy <run_dir> -t Bond Angle Proper-Dih.
```

ML models increase reaction task time

```
kimmdy-analysis runtime <run_dir>
```

Runtime of alanine_hat_021; overall 67.0 s

System generation is semi-automated

```
pepgen A ala/
```

System generation is semi-automated

```
kimmdy-remove-hydrogen pep.gro topol.top 14 -p -e
```

Conclusion

- KIMMDY v2 is mostly done
- All aspects of the reaction functionality have been revisited
- Theoretical foundations of KIMMDY are clear
- Practicality of these simulations remains to be shown

Thank You!