MD and Reactions

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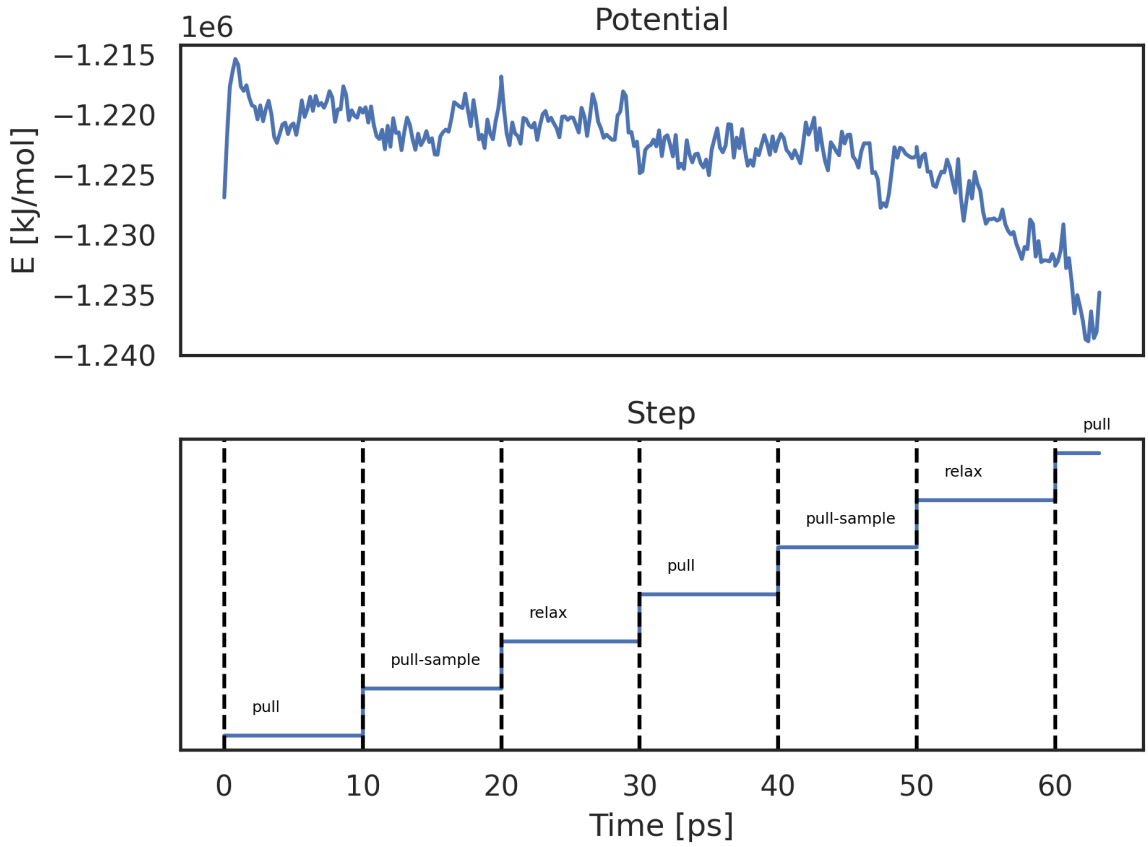
KIMMDY structure and theory

Practice

KIMMDY can break a triplehelix (and continue simulating for a bit)

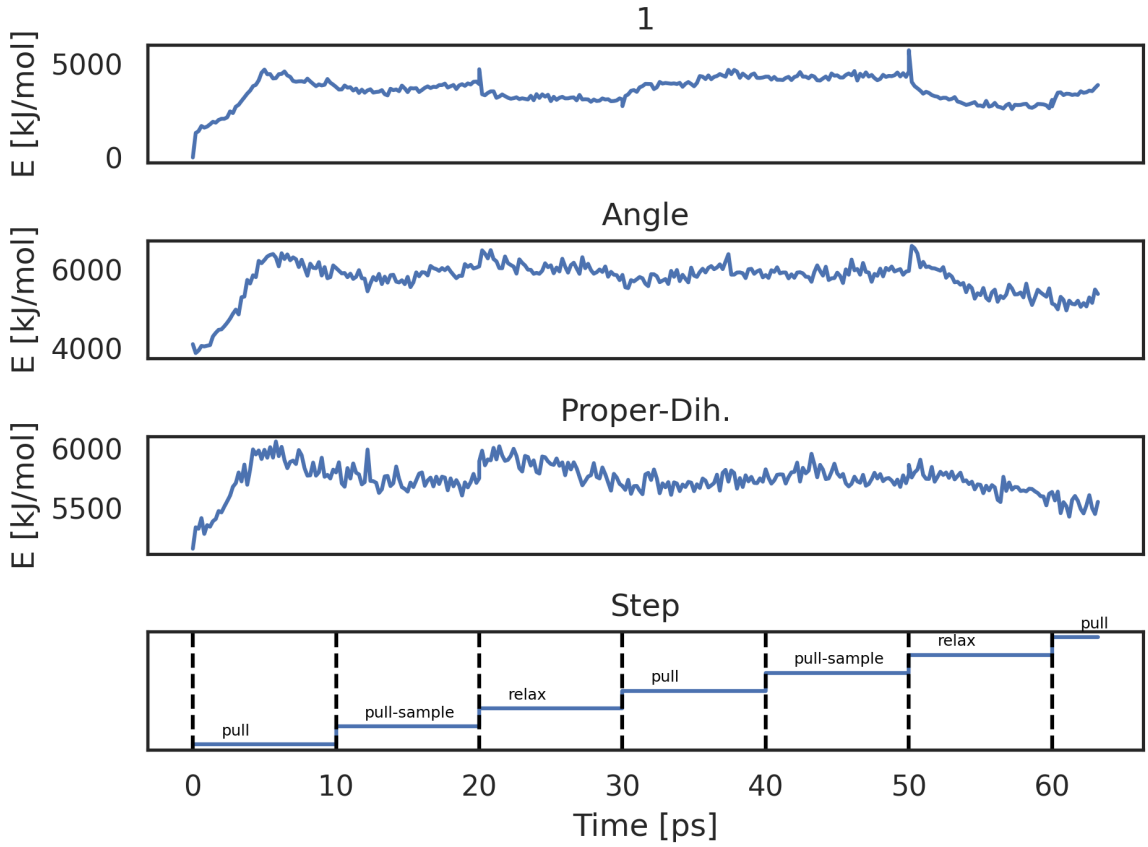
System energy is continuous

```
kimmdy-analysis energy <run_dir> -t Potential
```



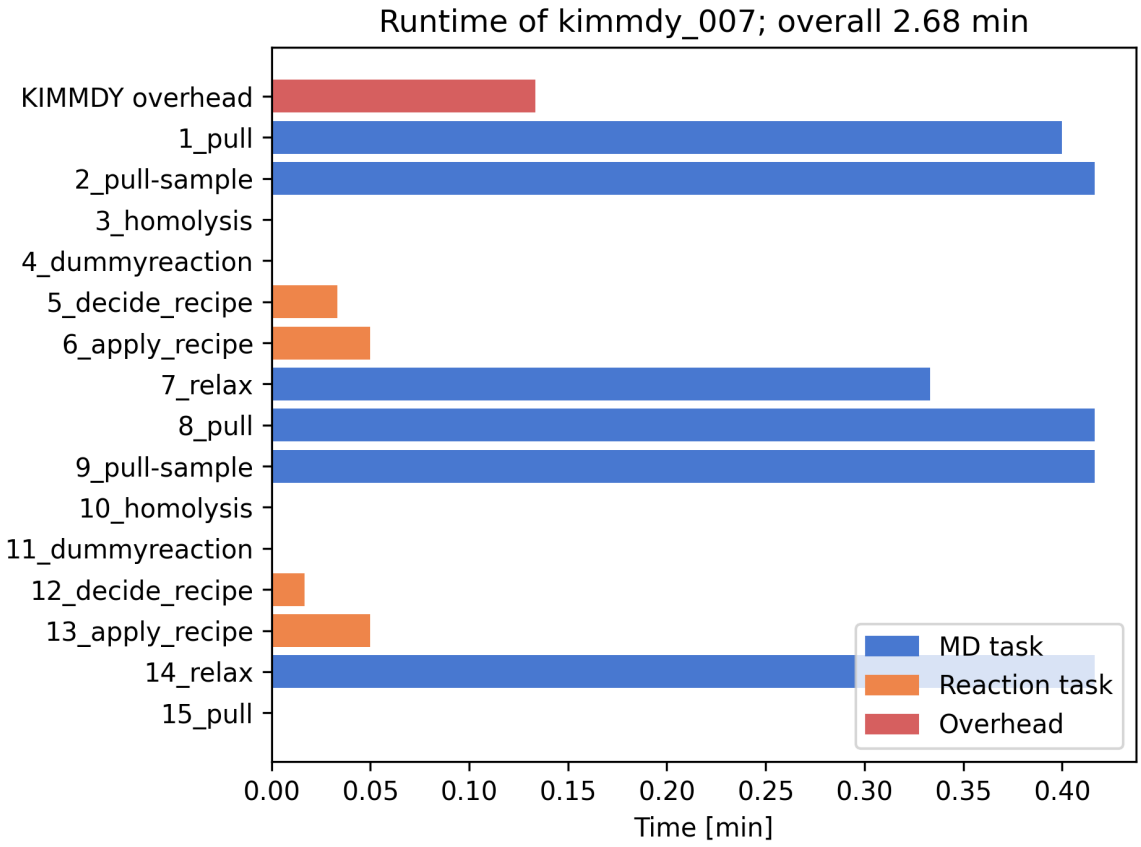
Intramolecular energy is continuous

```
kimmdy-analysis energy <run_dir> -t 1 Angle Proper-Dih.
```



Most of the time is spend on MD

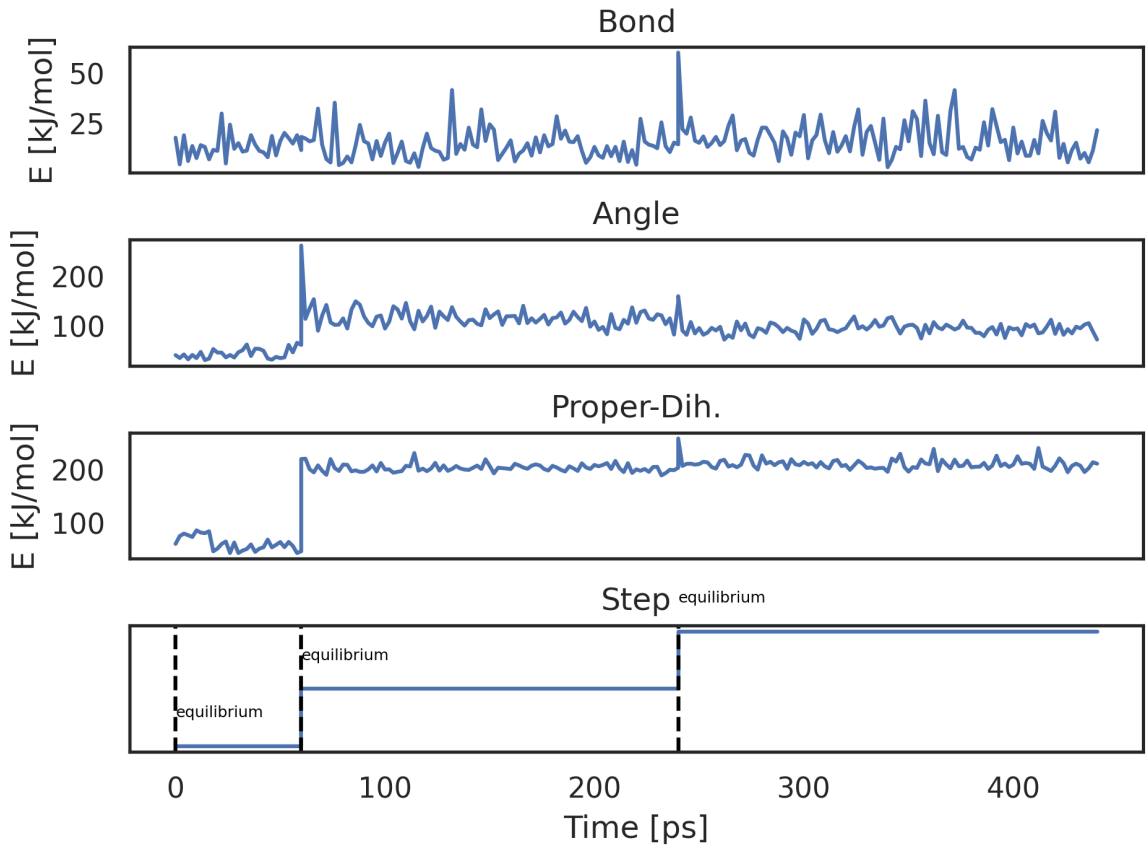
```
kimmdy-analysis runtime <run_dir>
```



KIMMDY can simulate HATs

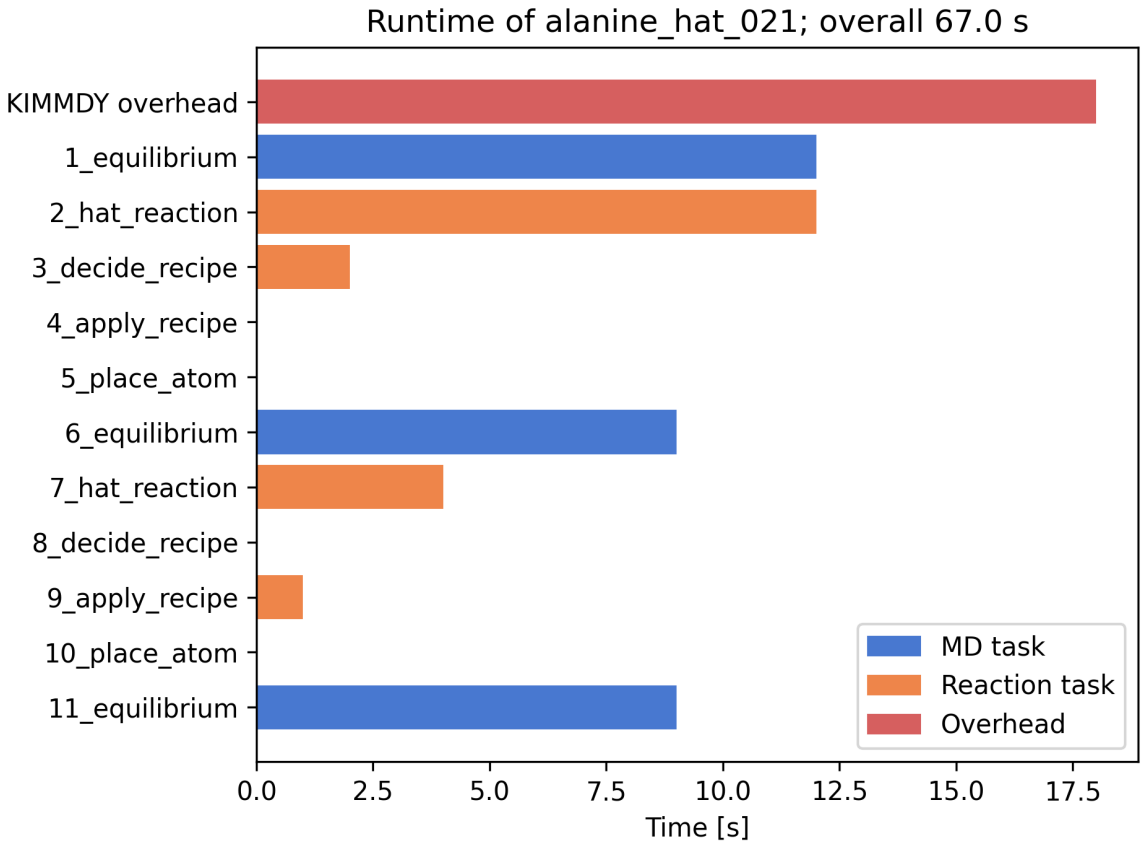
Intramolecular energy behaves almost physically correct

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



ML models increase reaction task time

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



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!