

Future Steps



What else could we implement in IMD v3?

(full description of current protocol: https://imdclient.readthedocs.io/en/latest/protocol_v3.html)

- communicate forces back to MD and guarantee synchronization (minimal change to IMD v2)
 - *e.g.*, enhanced sampling simulations
- modify atom coordinates/velocities/box in simulation
 - *e.g.*, hybrid Monte Carlo
 - prototyping new thermostats/barostats
- multiple parallel streams
- ...

What else would be interesting for you?

