Chore: Brute Force Bounties

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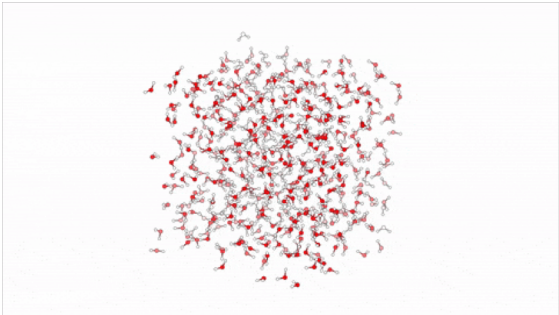
Objective

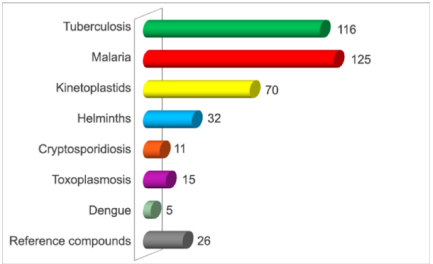
Molecule interactions can be approximated with simulations in OpenMM.

These simulations are computationally intensive, so we want to distribute the workload and reduce repeated work.

We would like a service where users can outsource jobs to other computers, with a nominal payout, and receive the results at a later time.

The system needs to receive job files, verify their integrity and feasibility, and make them available to clients.





Approach

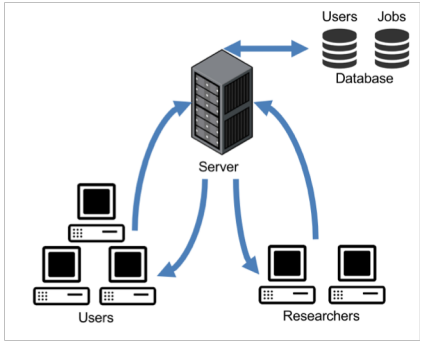
Publish-Subscribe Bounty Server:

Users register to the bounty server and can post jobs or fulfill jobs

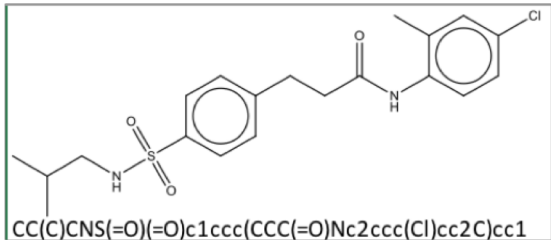
Jobs with the highest payout are given out until they are completed

Results are accepted after a validation period where other users can refute a submitted solution

Client is a Conda environment that seamlessly send/receives jobs from the server



Methods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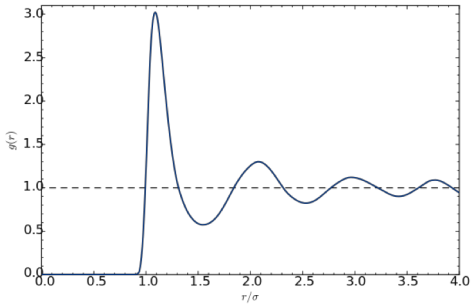
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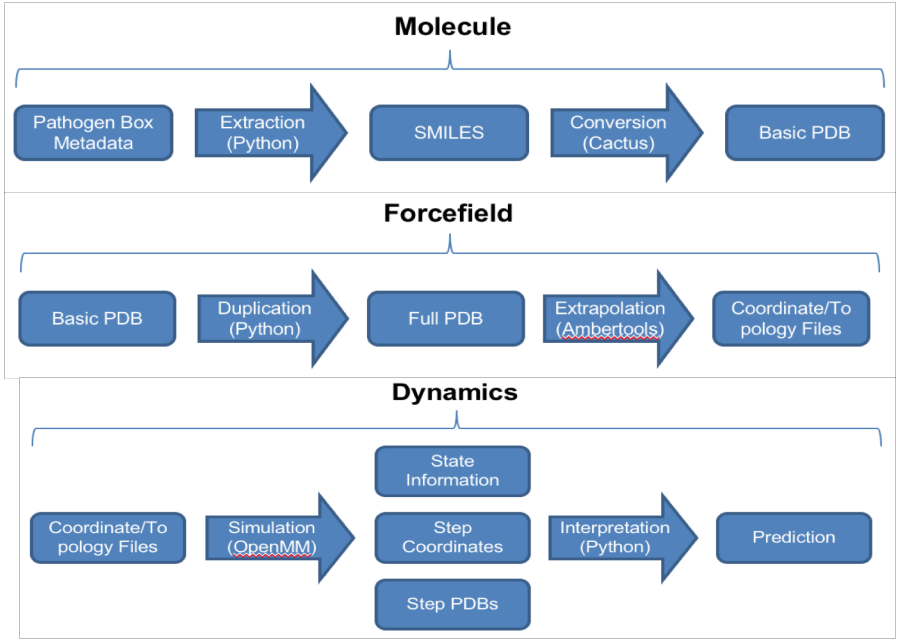

Molecule
Pathogen Box Metadata
Extraction (Python)
SMILES
Conversion (Cactus)
Basic PDB
Forcefield
Basic PDB
Duplication (Python)
Full PDB
Extrapolation (Ambertools)
Coordinate/To pology Files
Dynamics
State Information
Coordinate/To pology Files
Simulation (OpenMM)
Step Coordinates
Interpretation (Python)
Prediction
Step PDBs

Schedule

Came up with a somewhat different idea in January

Pared down our overly-ambitious idea in February

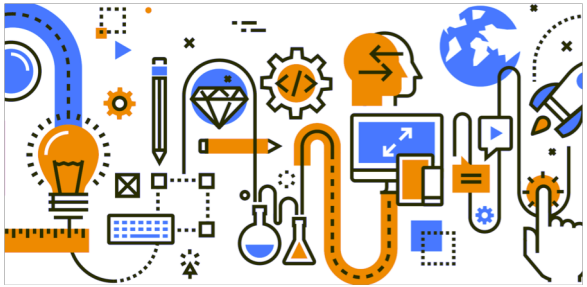
Started workflow 12 weeks ago (4 hours/week)

Started server 4 weeks ago (4 hours/ week)

Started client 4 weeks ago (2 hours/week)

Future Directions

- Security:
  - Ensuring job feasibility
  - Validation without re-computation
  - Secure client against potentially malicious jobs
- Generalization:
  - New job types
- Workflow:
  - Improve molecule descriptions
  - Use appropriate simulation settings/standards



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