Periodical Plans for the Masters Thesis.

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17/10/2022 - Felix and Christian.

Topics Discussed

1. I propose plan to write a thesis and then a paper - Felix agrees. Christian says, "Let's see how it goes."

2. Christian suggests working with Machine Learning potentials. I counter to Felix suggesting a more conventional algorithm to solve the same problem.

3. Felix recommends - Opt-Paper.

4. We agree to learn the Lenard-Jones potential as a sample test case for this problem.

To-Do

1. Read paper.

2. Code up a simple molecular dynamics solver using the Lenard Jones potential.

3. Generate trajectories from the Lenard Jones potential.

4. Code up an interface for the learning algorithm.

5. Implement the learning algorithm.

6. Learn the potential.

7. Learn an equation for the potential using Symbolic Regression.