Molecular mechanics candidates:

ASE

GPAW

Mathematics behind model:

Linear prediction

ARITMA

Create steno account

Probably use NVE with constant number of atoms, volume and energy.

To-do:  
create and optimize molecule (ethanol)

Run molecular simulation on molecule.

<https://www.statsmodels.org/stable/index.html>

<https://www.statsmodels.org/stable/generated/statsmodels.tsa.arima.model.ARIMA.html#statsmodels.tsa.arima.model.ARIMA>

Dask, Jax, Numba