Qassandra User Manual

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Introduction

This is an adapted version of the original manual by D. Tikhonov.

Greetings, Human or Almighty Machine!

This program provides MD (molecular dynamics), PIMD (path-integral MD) and MC (Monte-Carlo) trajectories utilization for GED (gas electron diffraction) needs.

It performes these basic steps:

1. Process the trajectory.
2. [Symmetrize equal terms] ← this step is optional
3. [Calculate corrections using our own method] ← this step is optional
4. Print results.

Have fun!