

R E A D M E

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- **This** is the first distribution of POST-PROMD: a POST-PROcessing software for all-scale/all-atom Molecular Dynamics (MD) simulations.
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- **Please**, refer to [1] for information about the mathematical relations used in POST-PROMD.
- **Written in:** Fortran 95 and Linux Bash
Operating System: Linux
Compatible with: Intel Fortran Compiler (ifort)
- **Purpose:** To compute three important phase transition indicators including: the Lindemann index, mean square displacement (MSD) of atoms, and radial distribution function (RDF) of systems of atoms/particles. Originally written to post-process the MD output file "cp.pos" generated by the CPV package of Quantum ESPRESSO (QE).
- **Input Files:** "cp.pos" and "par.input"
- "par.input": Contains a number of numerical parameters as follows:
n0 = Total number of particles.
nstep0 = Total number of steps.
iprint0 = Number of steps between successive output writings (included in MD input file of QE).
ign0 = Number of steps for thermalization/thermal equilibration, usually between 50 and 500 steps, to have reliable statistical averages.
dt0 = Time-step included in (1st row, 2nd column) of "cp.pos".
dt00 = Time-step in MD input file of QE.
delta_r0 = Increment value in radius r ; 0.0005 Å works well.
rmax0 = Distance from COM to the outermost shell of the system; Example: 5 Å for B₃₆ nanocluster[2].

- **Details:**

- **lind.sh:**

- Purpose: Computes the Lindemann index (Δ_{rms}).

- Input files: "cp.pos" | "par.input" | "ln.source"

- Output file: No file

- **msd.sh:**

- Purpose: Computes mean square displacement of every atom/particle of the system.

- Input files: "cp.pos" | "par.input" | "msd.source"

- Output files: "msd***.out" contained in directory <msd_output_files>. The user has to plot the output files, each containing 2 columns of data: time-step and MSD.

- **rdf.sh:**

- Purpose: Computes radial distribution function (RDF) of systems of atoms/particles

- Input files: "cp.pos" | "par.input" | "rdf.source"

- Output file: "rdf5.out" contained in directory <rdf_output_file>, including 5 columns: r, rdf on xy plane, rdf on xz plane, rdf on yz plane, and rdf in three dimensions. The user also has to plot this file.

- **How to Run:**

- 1- Unzip POST-PROMD compressed file `post-promd-v.1.0.0.tar.gz`.

- 2- Place "cp.pos" in the directory <src>.

- 3- Edit "par.input" according to your MD setup, then place it in <src>.

- 4- Open a terminal in the directory <src>.

- 5- To compute Lindemann index, run in terminal: `bash lind.sh`.

- 6- To compute MSD, run in terminal: `bash msd.sh`.

- 7- To compute RDF, run in terminal: `bash rdf.sh`.

- **Example File:** This distribution contains an example files related to MD simulation of the unit cell of SLSiN (single-layer Si_3N_4), containing 14 atoms, within the Car-Parrinello approach, at $T = 5$ K. For more information on SLSiN, please refer to [3].

- **Version:** v.1.0.0

- **Compressed File Name:** post-promd-v.1.0.0.tar.gz

- **Logo:** Rendered in <https://app.logo.com>.



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- **QR Code:** To quickly download via mobile phone/tablet.

