# R E A D M E

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- **This** is the first distribution of POST-PROMD: a POST-PROcessor package for all-scale/all-atom Molecular Dynamics (MD) simulations.
- **Programmer:** Ashkan Shekaari
**Primary Email:** shekaari.theory@gmail.com
**Secondary Email:** shekaari@email.kntu.ac.ir
**Social Link:** `https://rt.academia.edu/AshkanShekaari`
**Orcid:** `https://orcid.org/0000-0002-7434-467X`
- **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 $B_{36}$ nanocluster[2].

- **Details:**
  - `lind.sh`:
    Purpose: Computes the Lindemann index (delta_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.