

"Theory of Local Sampling (TLS)" codes developed by Sahasrara Research (www.sahasrararesearch.in)

Notes:

1. As open-source initiative, users are requested to share your contributions and we share it in www.sahasrararesearch.in. Please contact us at shanmugam138@gmail.com
2. All codes were written in Fortran language.
3. Main file name is md.f90 (for Molecular dynamics algorithms) and mc.f90 (for Monte Carlo algorithms).
4. Corresponding module files used can be found in md.f90 and mc.f90 files.
5. Makefile was not included in the download folder and users are requested to create their own Makefile by looking into md.f90 or in mc.f90 files.
6. For Conventional MD simulation, module file for calculating of potential, force acting and acceleration acting on particles is acc.f90
7. To know more about "Theory of Local Sampling (TLS)", read paper/preprint titled "Theory of Local Sampling: An Effective Sampling Technique in Monte Carlo and in Molecular Dynamics Simulations with achieved Reduction in Computation Time up to 67%"

Hope it helps and have fun in your research studies!

For more information, visit www.sahasrararesearch.in or contact at shanmugam138@gmail.com