UANL

UNIVERSIDAD AUTÓNOMA DE NUEVO LEÓN

FCFM

FACULTAD DE CIENCIAS FÍSICO MATEMÁTICAS

UNIVERSIDAD AUTÓNOMA DE NUEVO LEÓN
FACULTAD DE CIENCIAS FÍSICO MATEMÁTICAS

Simuladores Moleculares

Nombre:
Giovanni Gamaliel López Padilla

Matricula:
1837522

5 de octubre de 2020

Palabras clave:

---

[1] David S. Cerutti, Robert Duke, Peter L. Freddolino, Hao Fan, and Terry P. Lybrand. A vulnerability in popular molecular dynamics packages concerning Langevin and Andersen dynamics. *Journal of Chemical Theory and Computation*, 4(10):1669–1680, 2008.

[2] Weinan E and Dong Li. The Andersen thermostat in molecular dynamics. *Communications on Pure and Applied Mathematics*, 61(1):96–136, 2008.

[3] Philippe H. Hünenberger. Thermostat algorithms for molecular dynamics simulations. *Advances in Polymer Science*, 173:105–147, 2005.

[4] M.S Shell. Advanced Molecular Dynamics. *Advanced molecular dynamics techniques*, pages 1–11, 2009.

[5] Simeon D. Stoyanov and Robert D. Groot. From molecular dynamics to hydrodynamics: A novel Galilean invariant thermostat. *Journal of Chemical Physics*, 122(11), 2005.