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Virialization of gravitational molecular dynamics systems and the impact of different pseudopotentials on the simulation. CESAR DIAZ, EDWIN TOMY GEORGE, ADRIAN DE LA ROCHA GALAN, JORGE MUNOZ, University of Texas at El Paso — The present work analyzes the behavior of two massive particles bounded in gravitational attraction, simulated using molecular dynamics techniques. When dealing with molecular dynamics simulations, it is often necessary to include an attenuated or increased force between the particles. This artificial force is called a pseudopotential, and in the case of this project, it is required to reduce as much as possible a problem of energy creation that occurs because the gravitational force tends to infinity when the objects are infinitely close to each other. The pseudopotential used is a changed version from Newton's Law of Gravitation, which includes a parameter called soften added to the denominator. This work tests different ways to calculate this soften parameter. The accuracy of each of the pseudopotentials is measured by a parameter called the virial factor. According to the classical mechanics' virial theorem, the result of this parameter is always -2 in nature. However, it was observed that the more negative the parameter is, the better the simulation conserves the energy of the particles. Preliminary results show this virial factor has maxima and minima in certain functions, and it is greater in magnitude when the time-step of the simulation is decreased.

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