Abstract Submitted
for the TSS21 Meeting of
The American Physical Society

Simulation and prediction of gravitational molecular dynamic systems, using diverse pseudopotentials and regression algorithms. EDWIN TOMY GEORGE, CESAR DIAZ CARAVEO, ADRIAN DE LA ROCHA, JORGE ALBERTO MUNOZ, University of Texas at El Paso — The present work simulates the dynamics of two gravitationally bounded bodies. This simulation is repeated with different initial conditions to generate data that is fed to regression models capable of predicting the future characteristics of the system with initial conditions, the objective being not needing to use time-consuming simulations for future calculations. The system itself consists of bodies in a one-dimensional space which are gravitationally attracted to each other, their masses, velocities and initial positions being the initial conditions. To accurately simulate the system, the use of pseudopotentials was needed to reduce the excess energy added when the particles come closer, caused by numerical errors that arise because Newton's Law of Gravity tends towards infinity in bodies that are infinitely close to each other. Different pseudopotentials were tested, comparing the accuracy of the simulation. The following modified Law of Gravity with the pseudopotential was selected, where lower variable lambdas are more accurate but time-consuming: GMm/(r^2+e^(-r/lambda)). After generating the simulations needed for the data, regression models where trained to predict different outcomes. A linear regression model was used to predict the final position of the particles, with a mean error of ~8%. A logistic model was used to predict if the system experienced collision or not. The next step on the present work is to use neural networks to improve the accuracy and implement more parameters.

Edwin Tomy George
University of Texas at El Paso

Date submitted: 24 Feb 2021 Electronic form version 1.4