

Supplemental material

Code of the NVERE method into implementation using the LAMMPS MD simulator:

```
variable p1 equal "step"
variable p2 equal "ke"
variable p3 equal "pe"
variable p4 equal "etotal"
fix 1 all nve
fix out all print 1 "${p1} ${p2} ${p3} ${p4}" file res-nve.txt screen
no
run 1
variable tmp equal ke
variable ke_old equal ${tmp}

label loop
variable a loop 30000
run 1
variable tmp equal ke
variable ke_new equal ${tmp}
if "${ke_new} < ${ke_old}" then &
"velocity all set 0.0 0.0 0.0 sum no units box" &
"variable ke_old equal 0" &
else &
"variable tmp equal ke" &
"variable ke_old equal ${tmp}"
next a
jump SELF loop
print "ALL DONE"
```