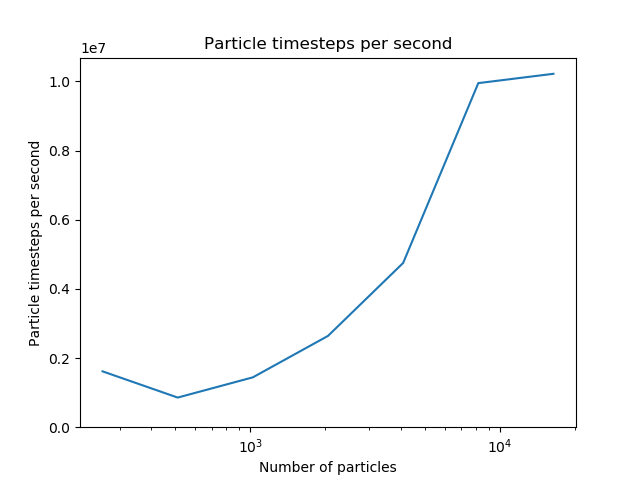
Exercise 4: molecular dynamics simulation

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Optimizations:

1. Make **accelerate\_indirect()** in a parallel region.

Graphical user interface

Description automatically generated with low confidence

1. Parallelize most for loops in **accelerate\_indirect()**, **bin\_particles()**, and **unbin\_particles()** with static schedule.



1. Collapse the triple for loop.

Text, letter

Description automatically generated

1. Apply nowait to velocity initialization because binning particles does not need velocity information.

Graphical user interface, text

Description automatically generated

1. In **bin\_particles()**, use atomic capture when updating **particle\_perm.**

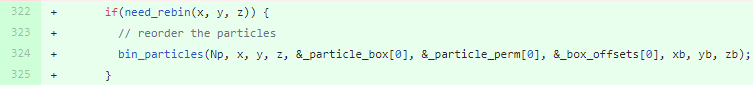


1. In **bin\_particles()**, keep prefix sum scan serial.

Text, letter

Description automatically generated

1. Add **need\_rebin()** function to only perform particle binning when necessary.



1. In **need\_rebin()** function, it will keep track of the particle positions from the last time the particles are binned, and calculate the maximum distance to decide whether particle binning is necessary. A parallel reduction for loop is used to calculate the maximum distance.

Text

Description automatically generated with medium confidence