

CHAPTER 19

Parallel programming and computational thinking

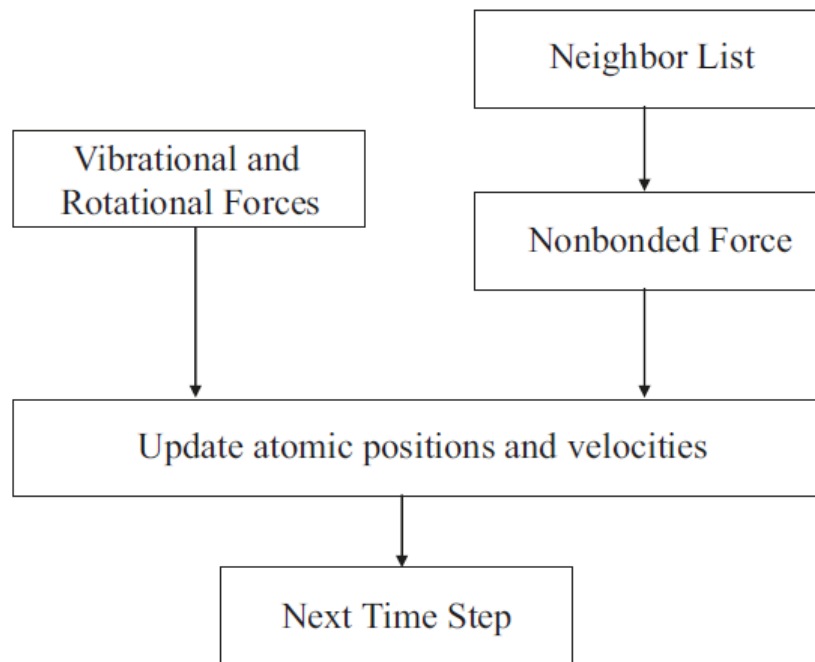


FIGURE 19.1

Major tasks of a molecular dynamics application.

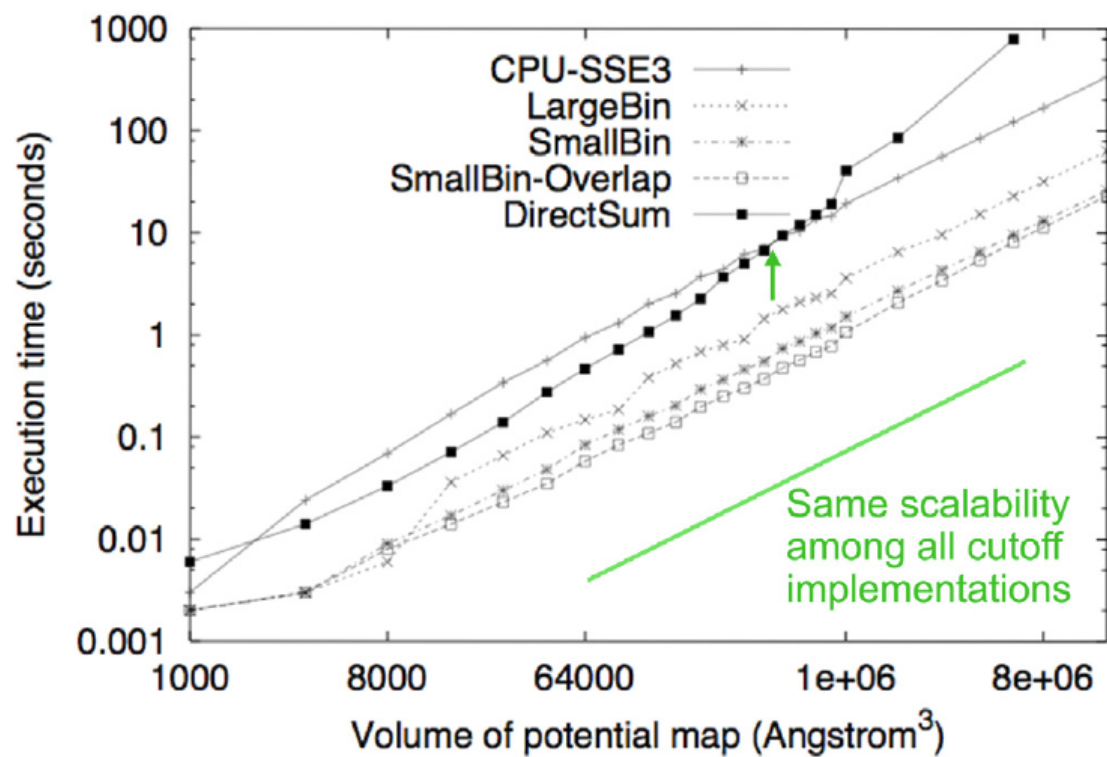


FIGURE 19.2

Scalability and performance of DCS versus cutoff binning.

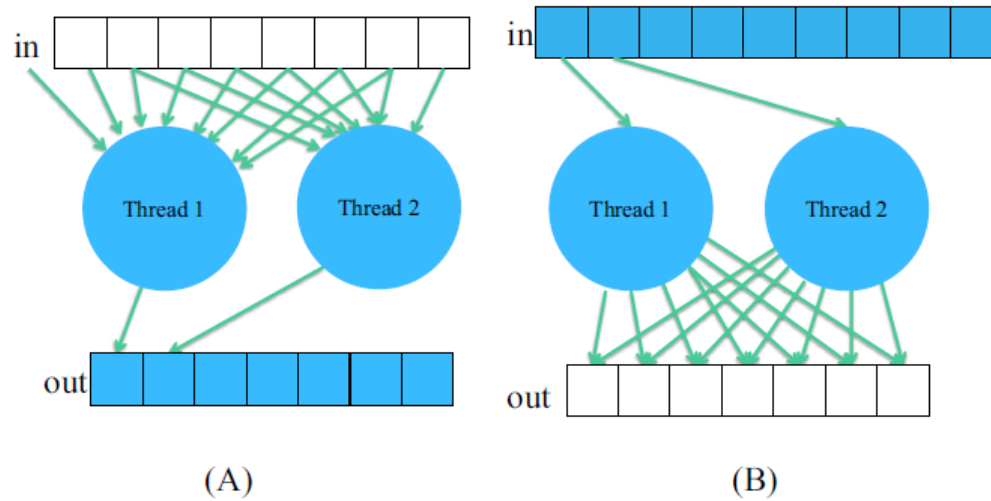


FIGURE 19.3

Problem decomposition strategies. (A) Output-centric. (B) Input-centric.