

Chapter-17

Parallel programming and computational thinking

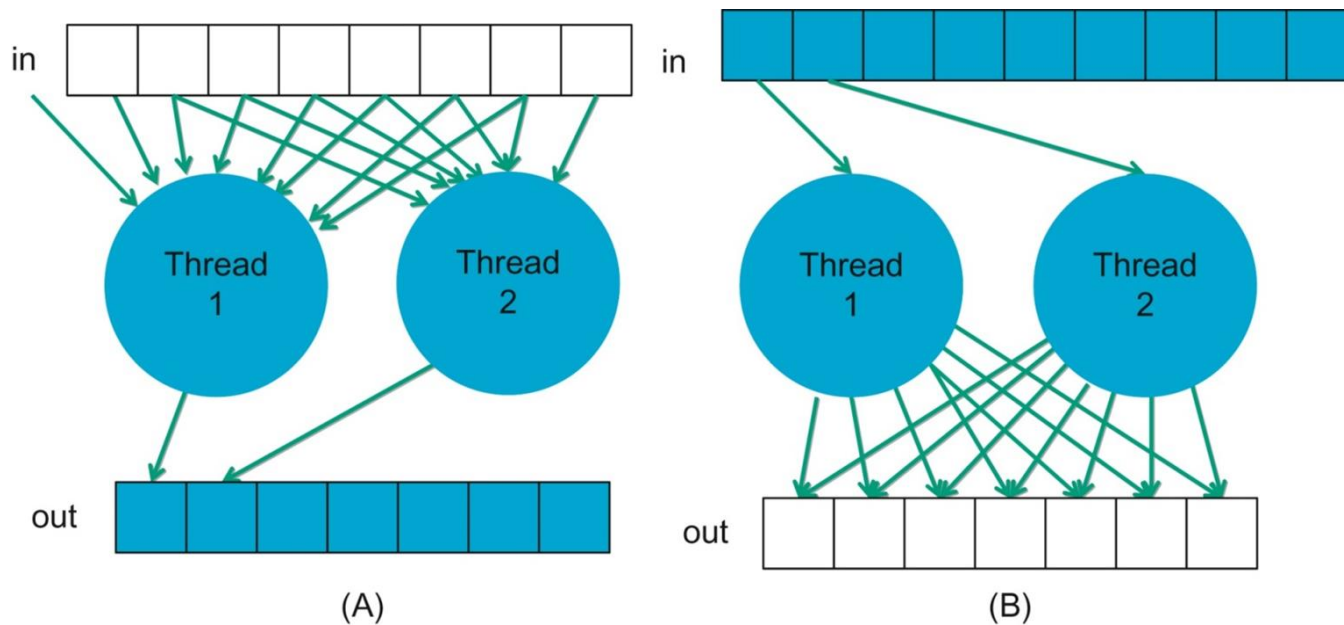


FIGURE 17.1: (A) Gather and (B) scatter based thread arrangements.

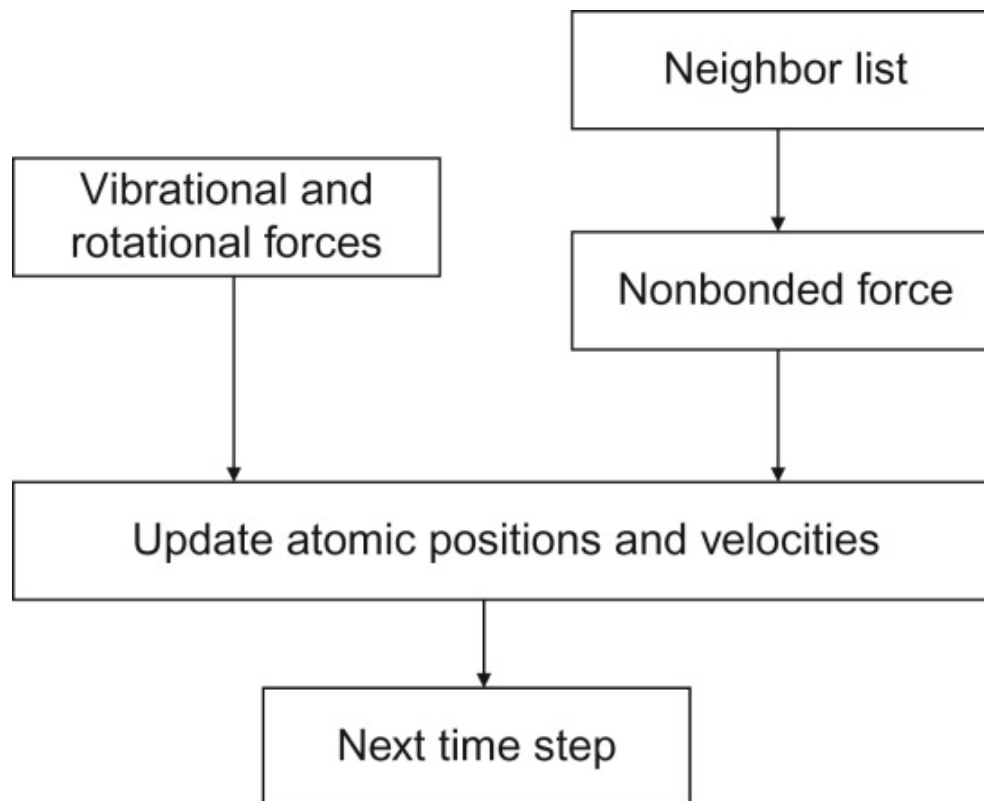
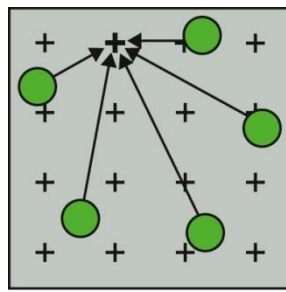
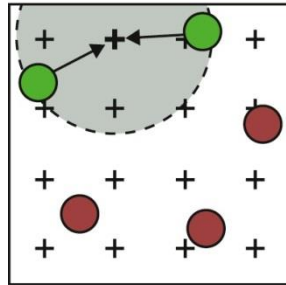


FIGURE 17.2: Major tasks of a molecular dynamics application.



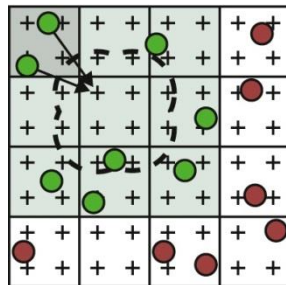
(A)

At each grid point, sum the electrostatic potential from all charges



(B)

Electrostatic potential from nearby charges summed; spatially sort charges first



(C)

Spatially sort charges into bins; adapt direct summation to process a bin

FIGURE 17.3: Cutoff summation algorithm. (A) Direct summation, (B) cutoff summation, and (C) cutoff summation using direct summation kernel.

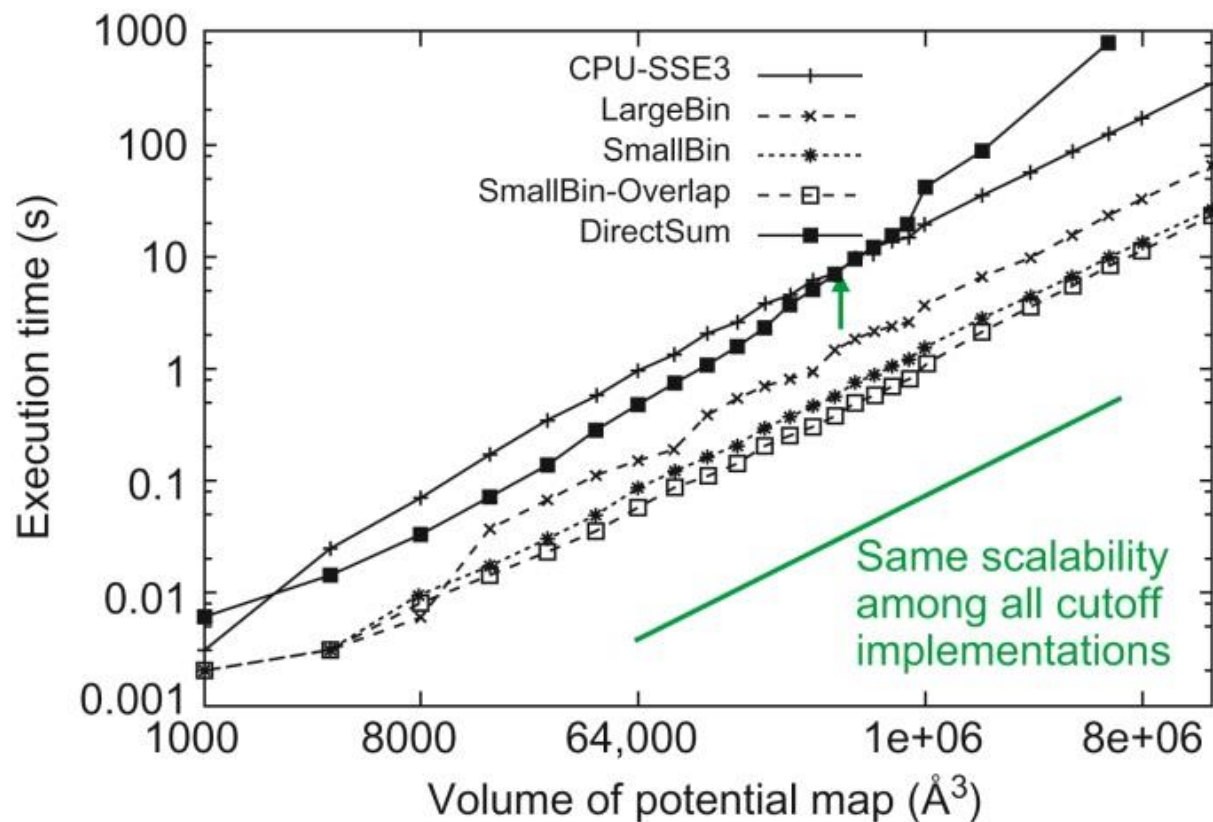


FIGURE 17.4: Scalability and performance of different algorithms for calculating electrostatic potential map.

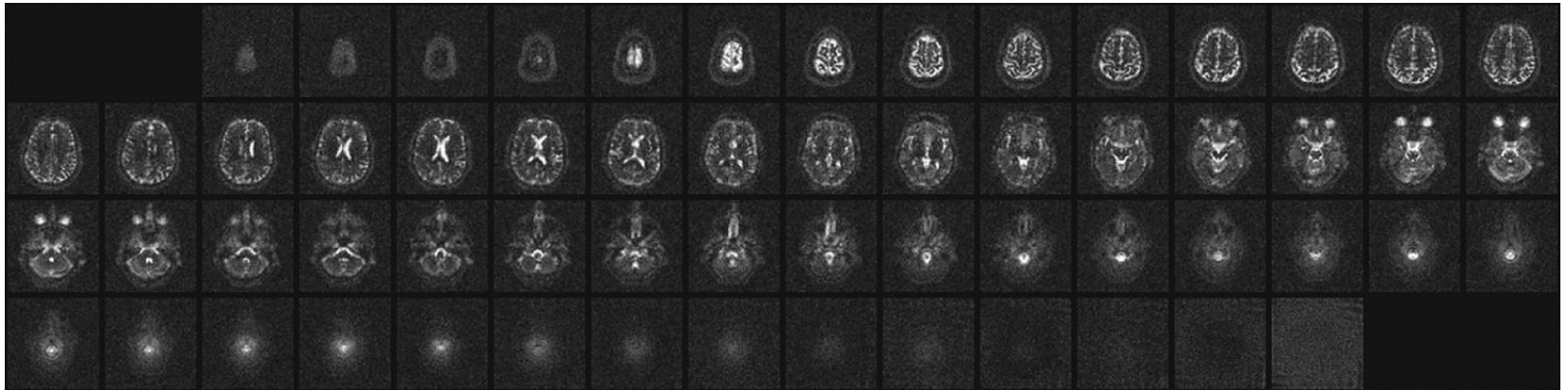
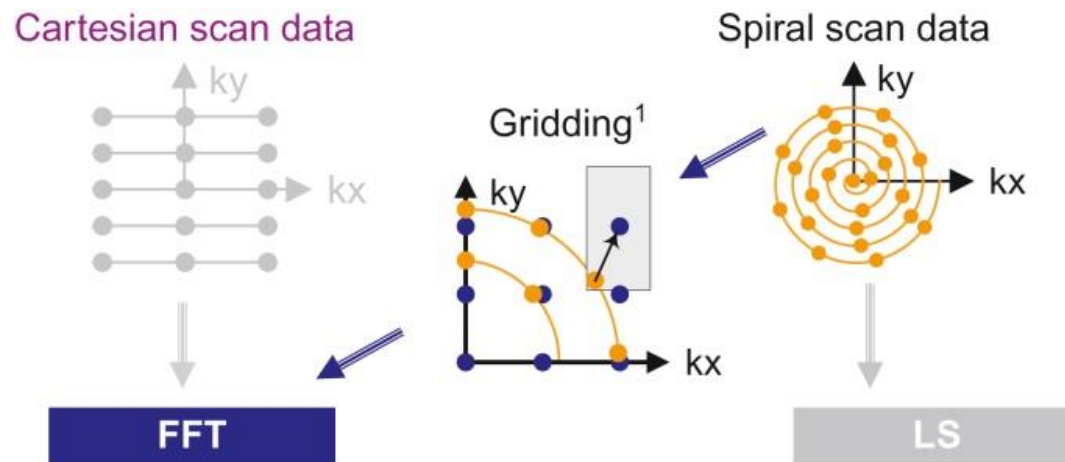


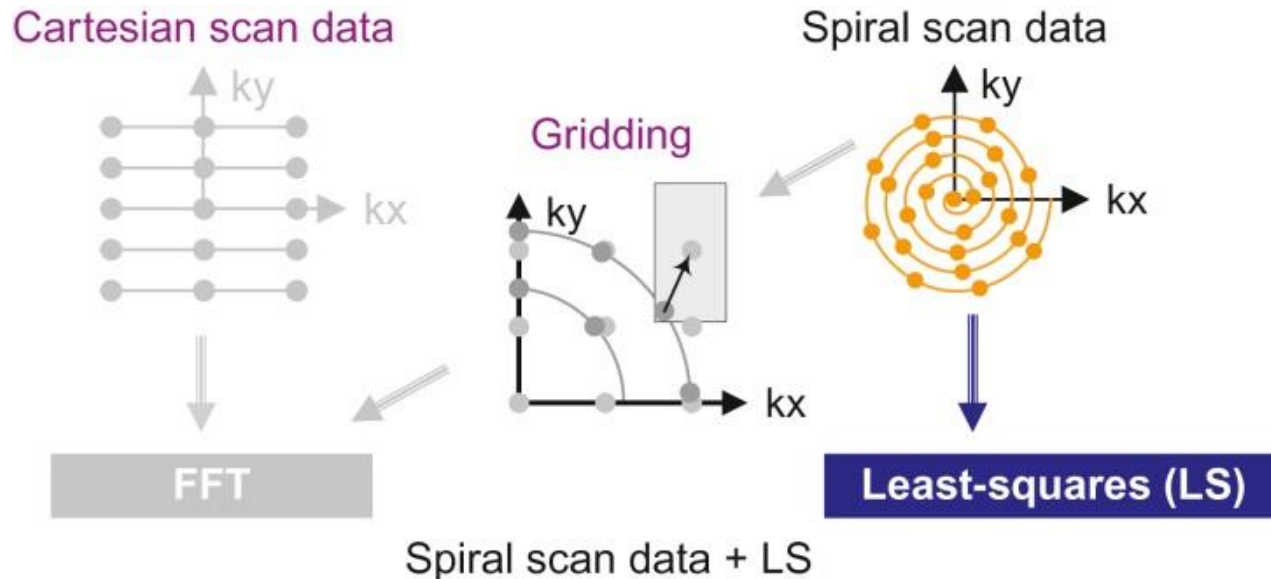
FIGURE 17.5: Sodium images of the brain. Courtesy of Keith Thulborn and Ian Atkinson, Center for MR Research, University of Illinois at Chicago.



Spiral scan data + gridding + FFT:
fast scan, fast reconstruction, good images
can become realtime with about 10X speedup.

¹Based on Fig 1 of Lustig et al. Fast Spiral Fourier Transform for Iterative MR Image Reconstruction, IEEE Int'l Symp. on Biomedical Imaging, 2004

FIGURE 17.6: Classical gridded MRI reconstruction from spiral scan data.



Superior images at expense of significantly more computation;
several hundred times slower than gridding.

Traditionally considered impractical!

FIGURE 17.7: Least squares reconstruction of spiral scan data.