Chapter-17
Parallel programming and computational thinking
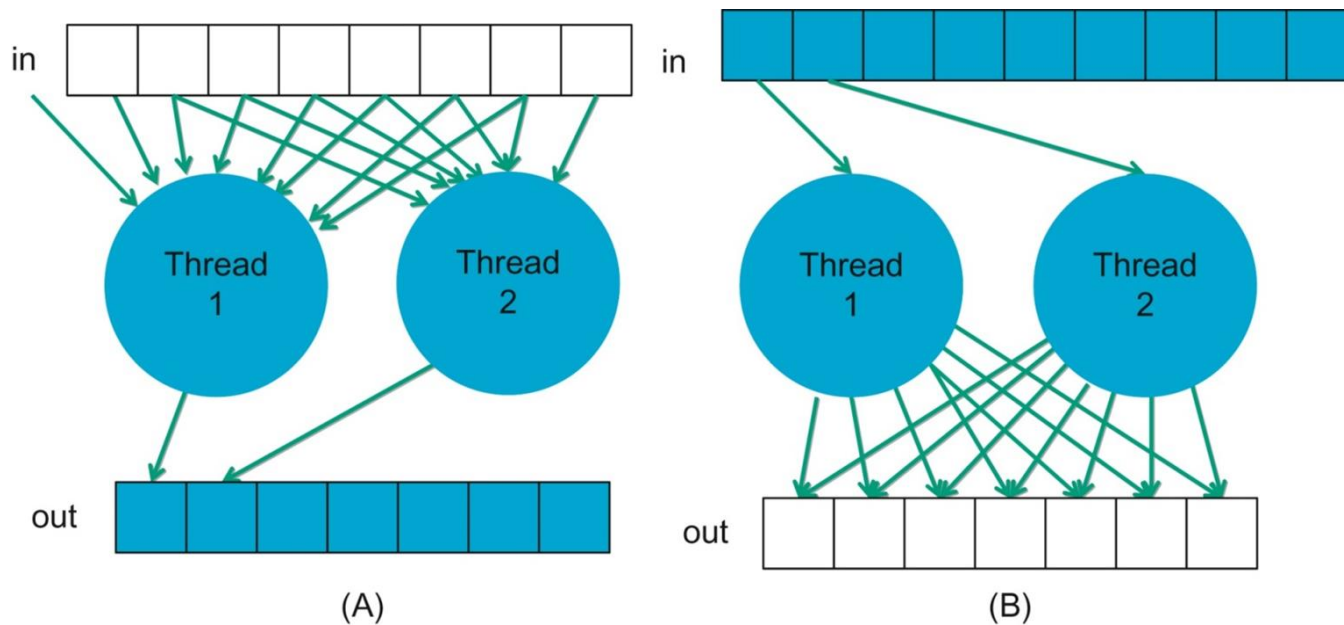
FIGURE 17.1: (A) Gather and (B) scatter based thread arrangements.
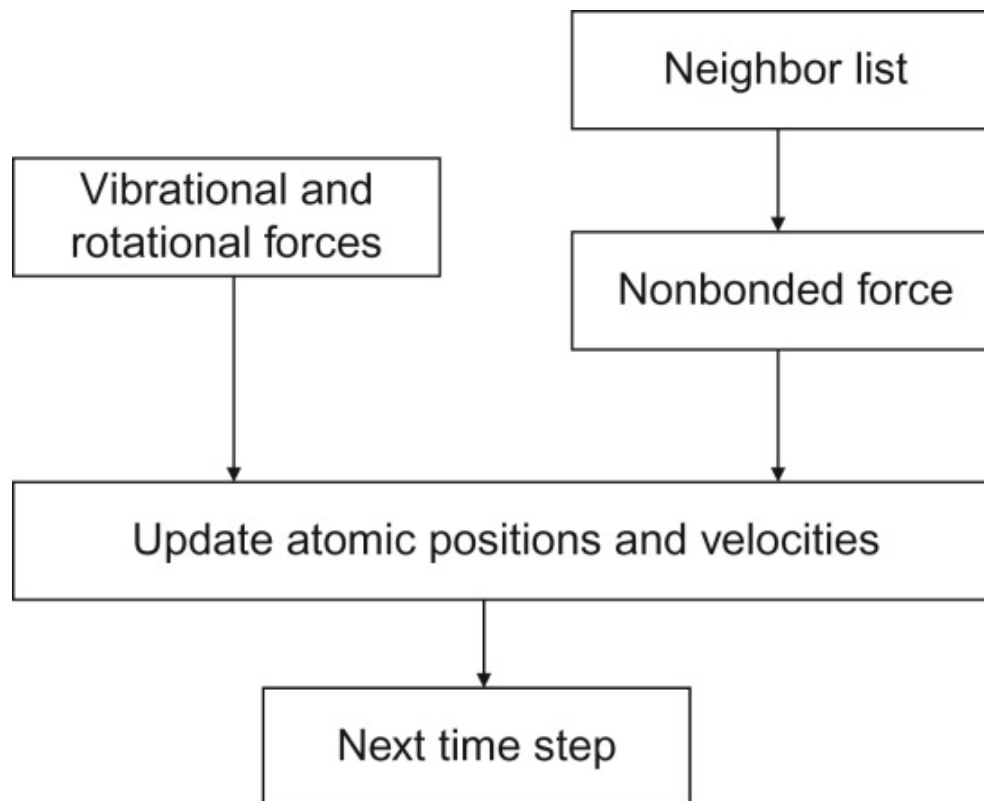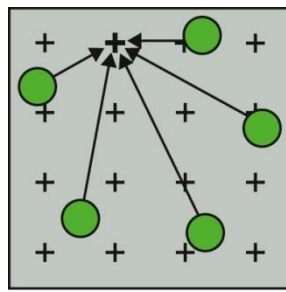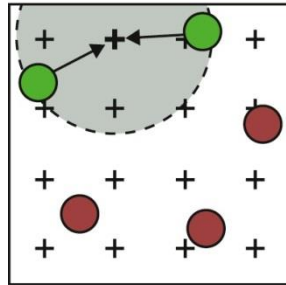
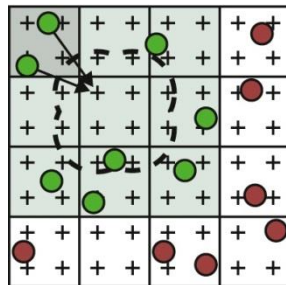**FIGURE 17.2**: Major tasks of a molecular dynamics application.

FIGURE 17.3: Cutoff summation algorithm. (A) Direct summation, (B) cutoff summation, and (C) cutoff summation using direct summation kernel.
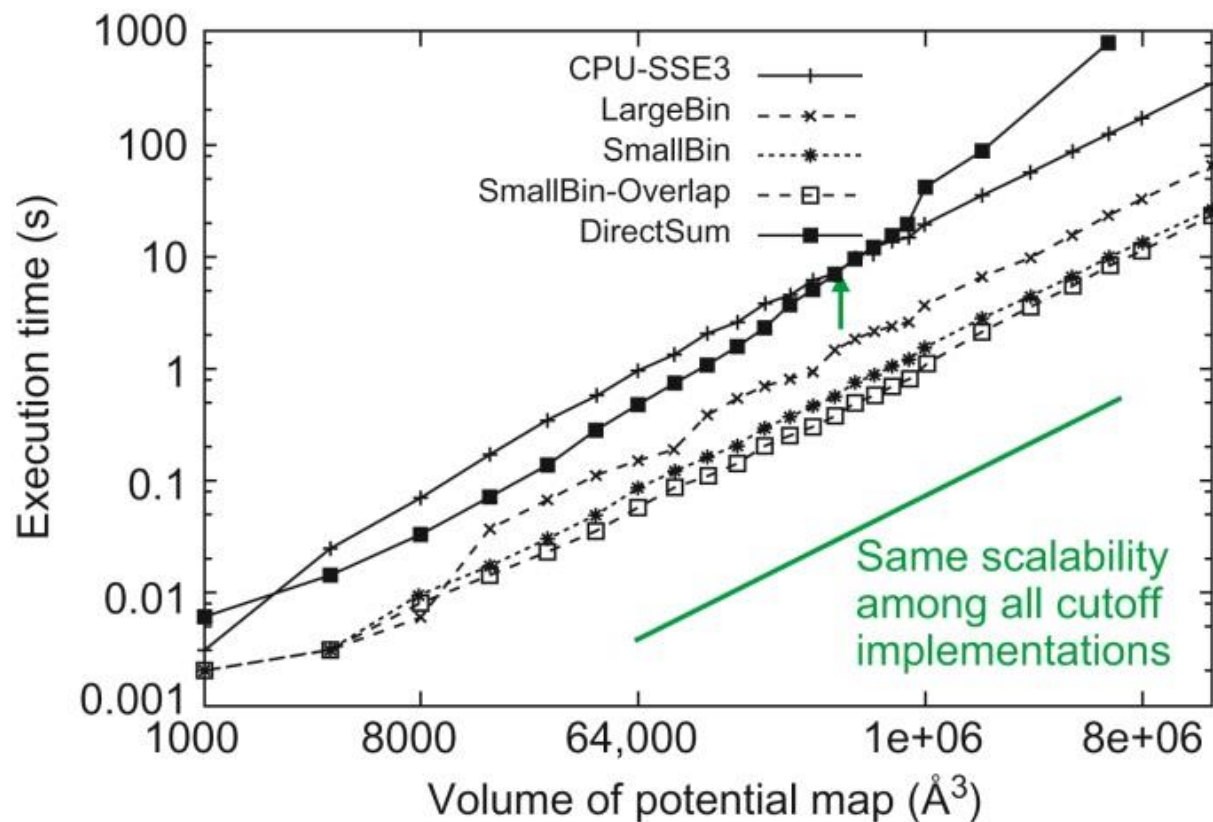
FIGURE 17.4: Scalability and performance of different algorithms for calculating electrostatic potential map.
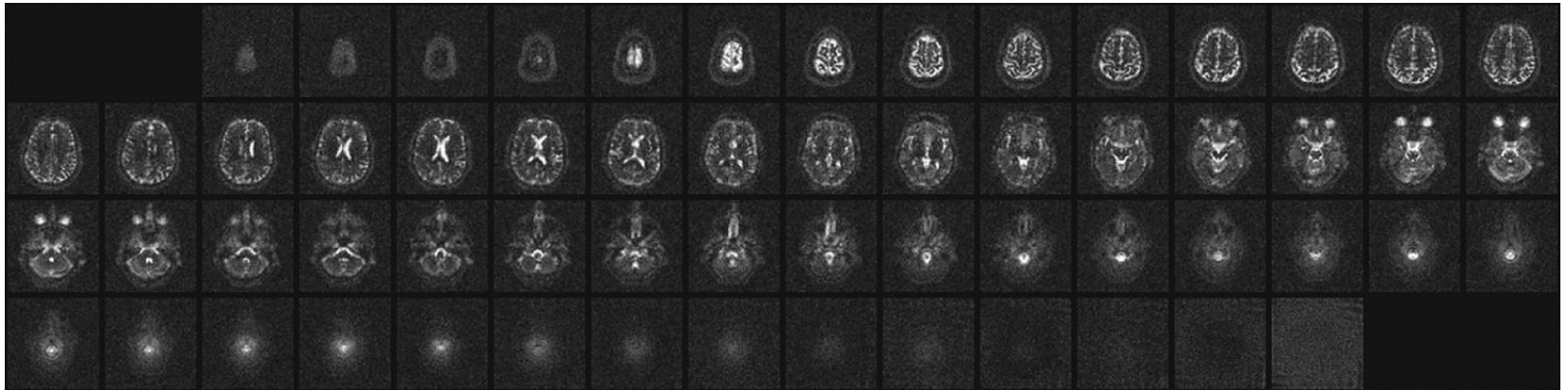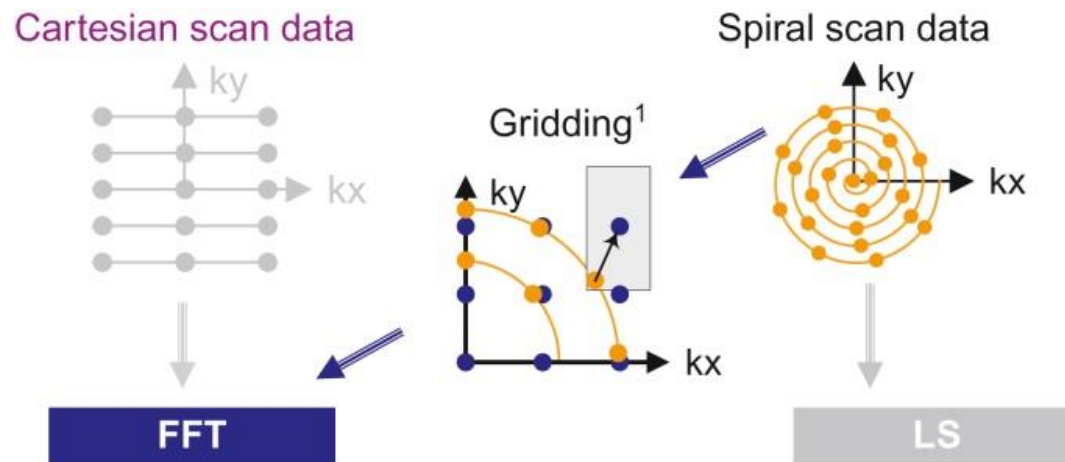
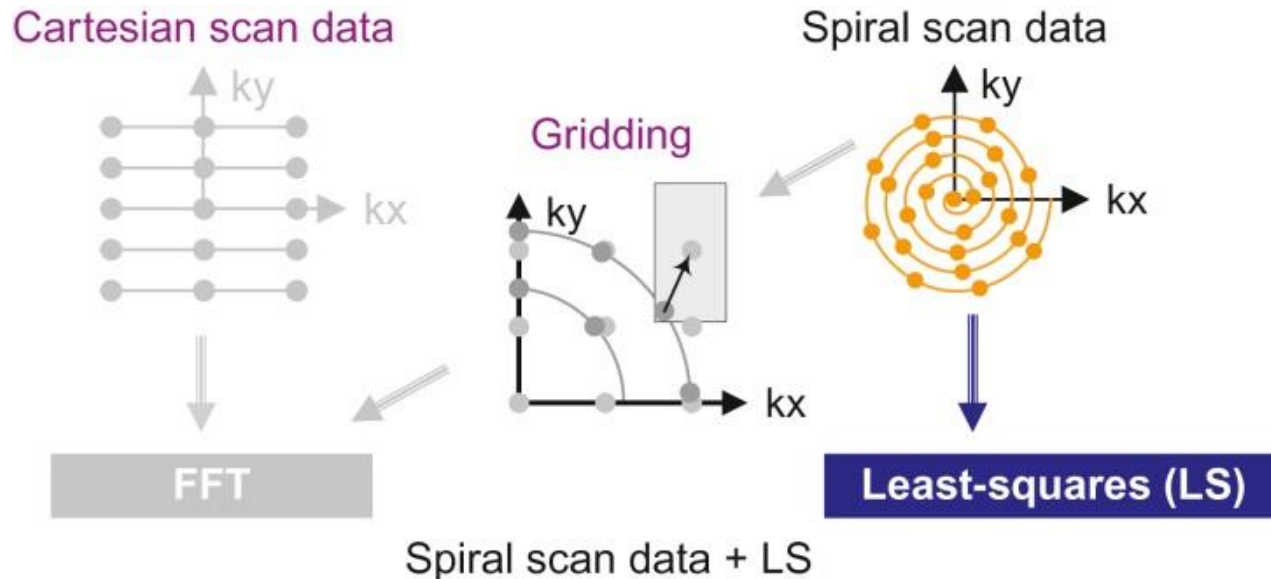**FIGURE 17.5**: Sodium images of the brain. Courtesy of Keith Thulborn and Ian Atkinson, Center for MR Research, University of Illinois at Chicago.

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

Cartesian scan data

ky

kx

Gridding

ky

kx

Spiral scan data

ky

kx

FFT

Least-squares (LS)

Spiral scan data + LS
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.