

Optimal Spatial Decomposition for MD Simulations

Draw the optimal spatial decomposition scheme for running MD simulations for the systems provided in Figure 1 using 10 cores and Figure 2 using 6 cores. Grid lines are shown as a guide to the eye. Assume the particles (not shown) are homogeneously distributed inside the walls.

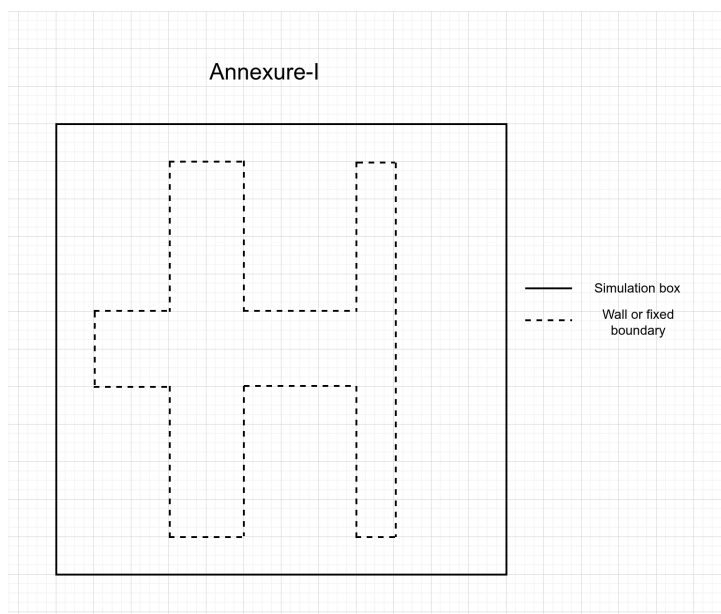


Figure 1: Spatial Decomposition using 10 cores

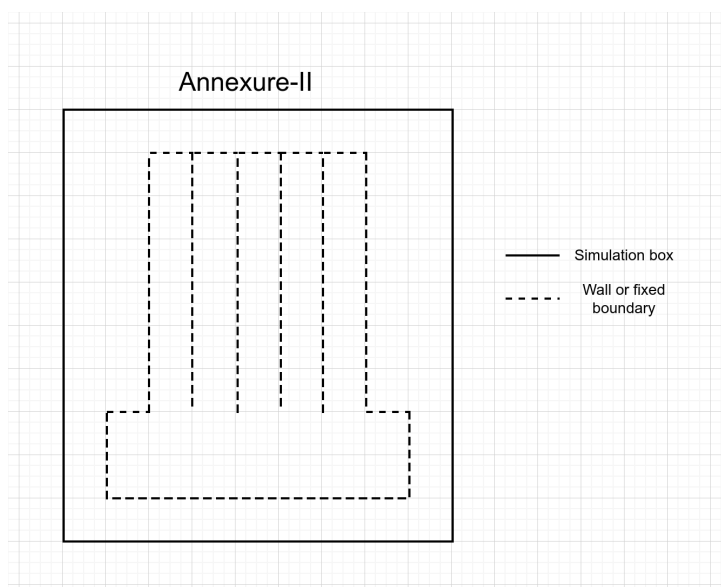


Figure 2: Spatial Decomposition 6 cores

Draw optimal spatial decomposition schemes for the two systems provided in both Figure 3&4 using 8 processors. Figure 3: The system consists of $12 \times 16 = 192$ atoms arranged in a square. Figure 4: The system consists of 52 atoms arranged in a square.

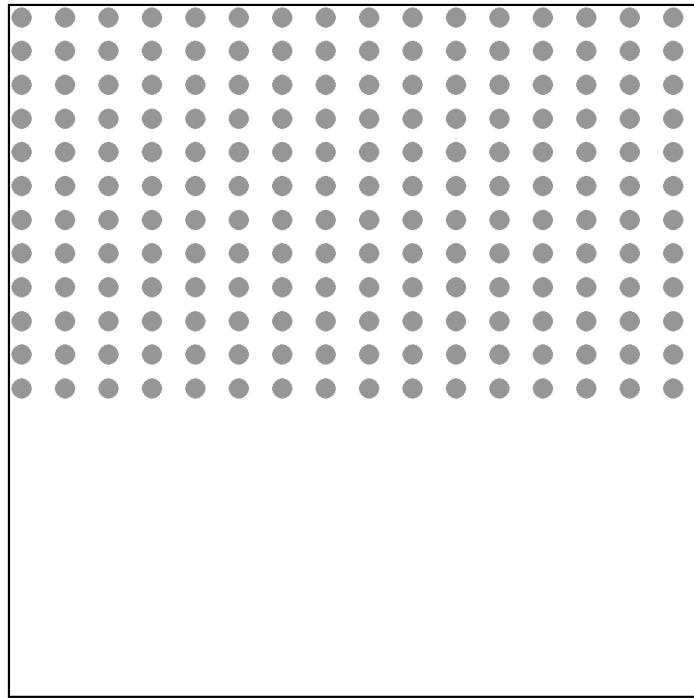


Figure 3: Spatial Decomposition 8 cores

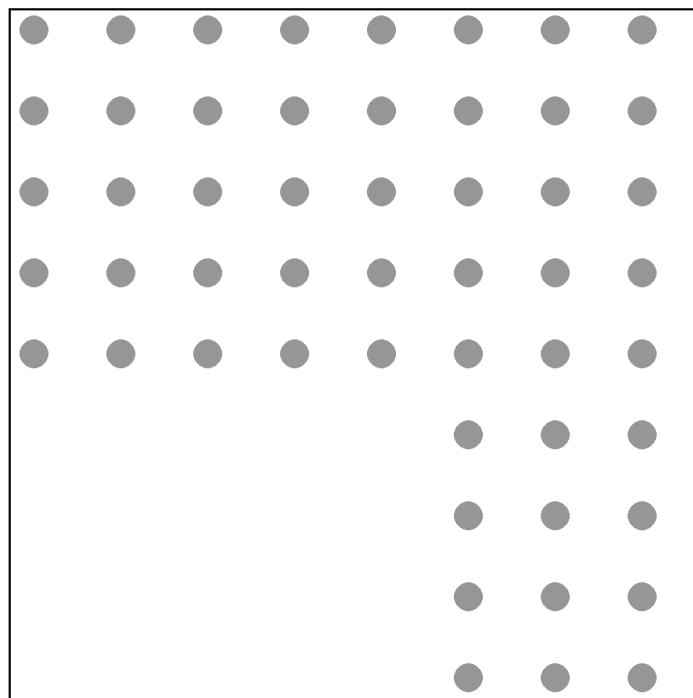


Figure 4: Spatial Decomposition 8 cores