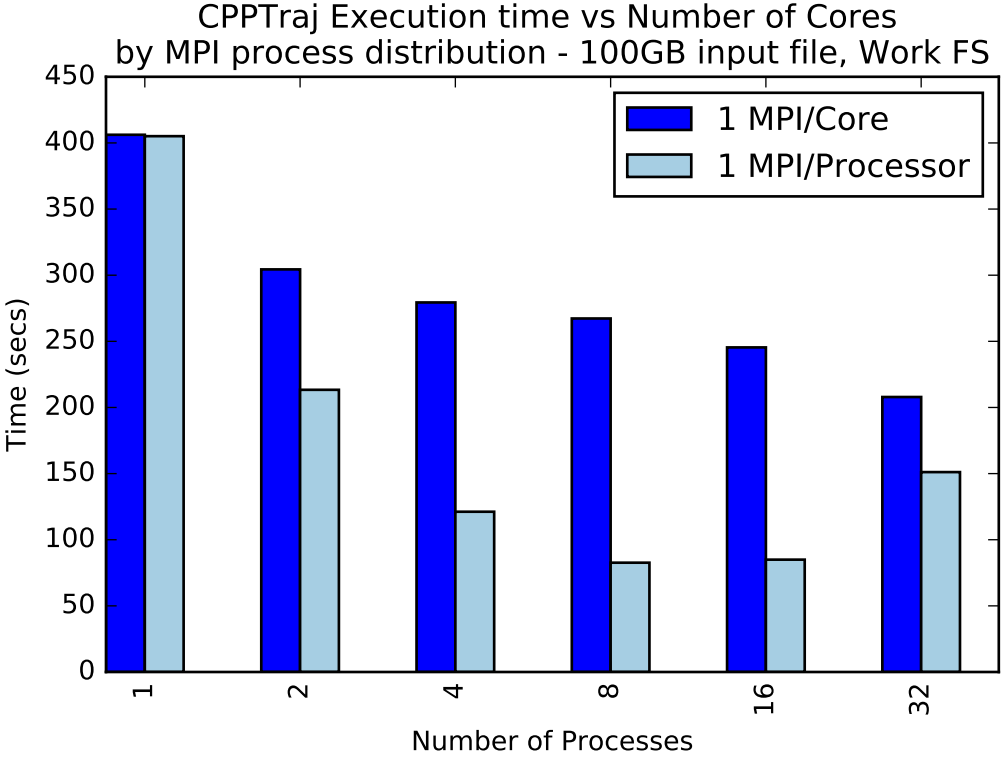
CPPTraj Execution time vs Number of Cores
by MPI process distribution - 100GB input file, Work FS
1 MPI/Core
1 MPI/Processor
Time (secs)
0
50
100
150
200
250
300
350
400
450
1
2
4
8
16
32
Number of Processes