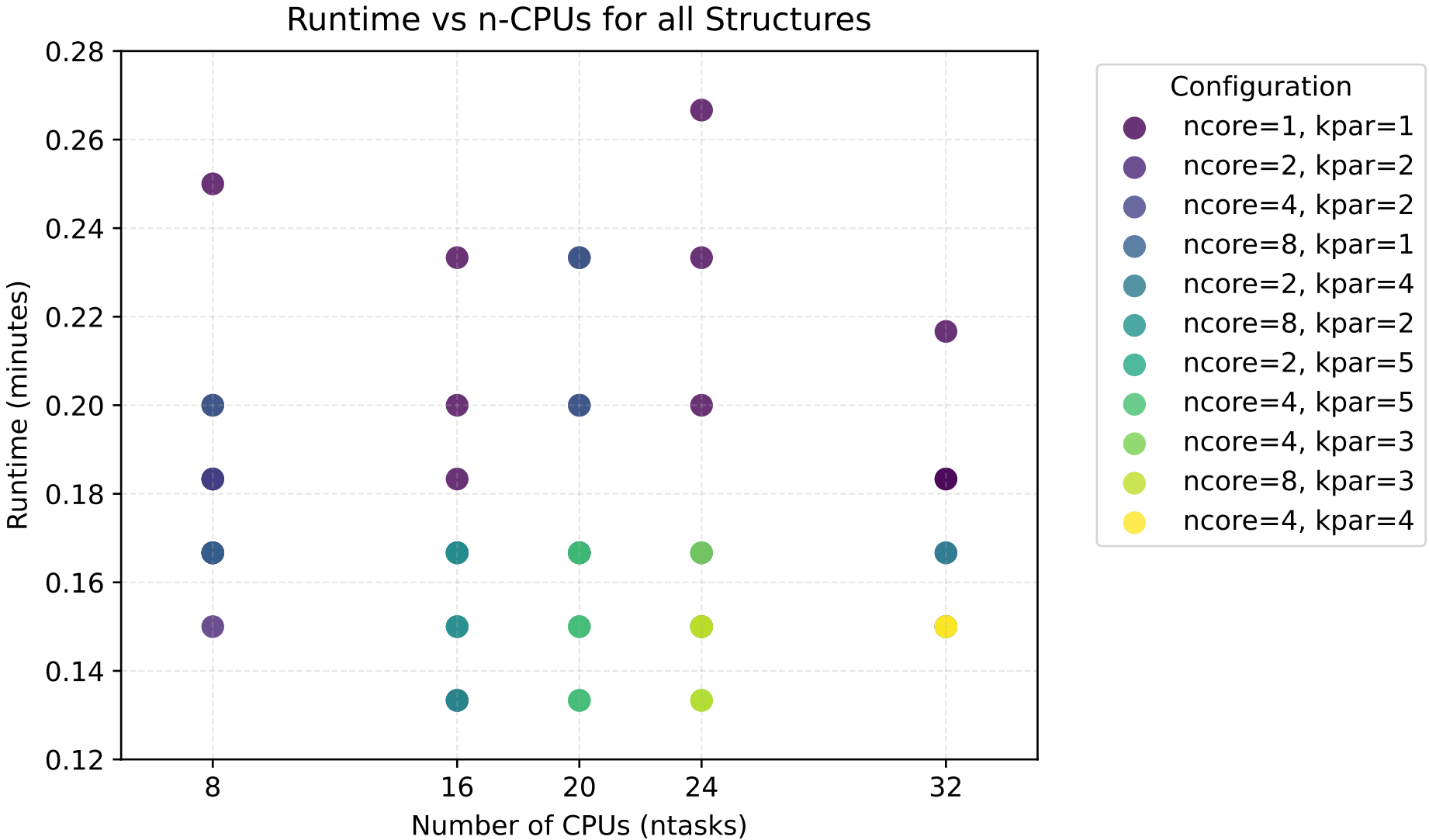
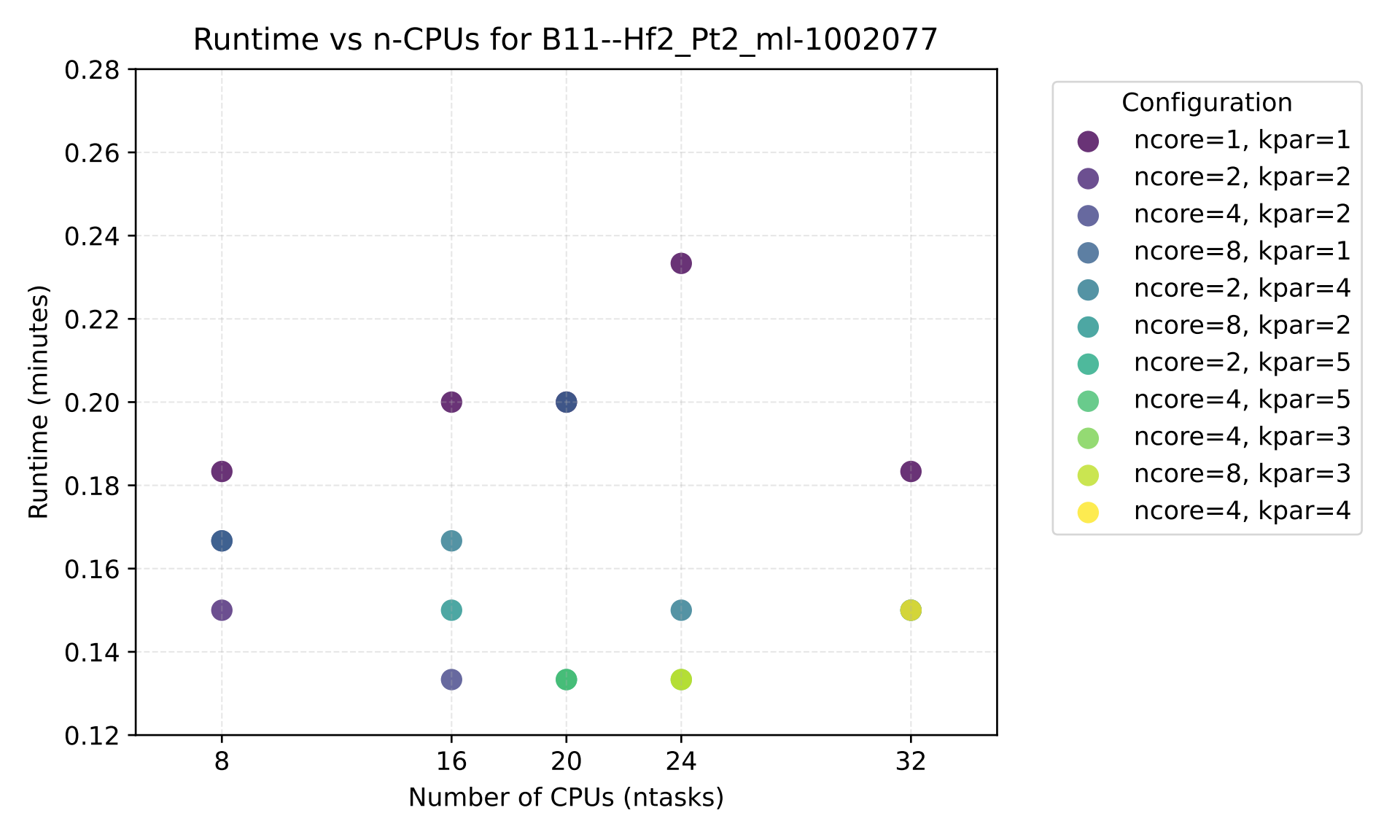
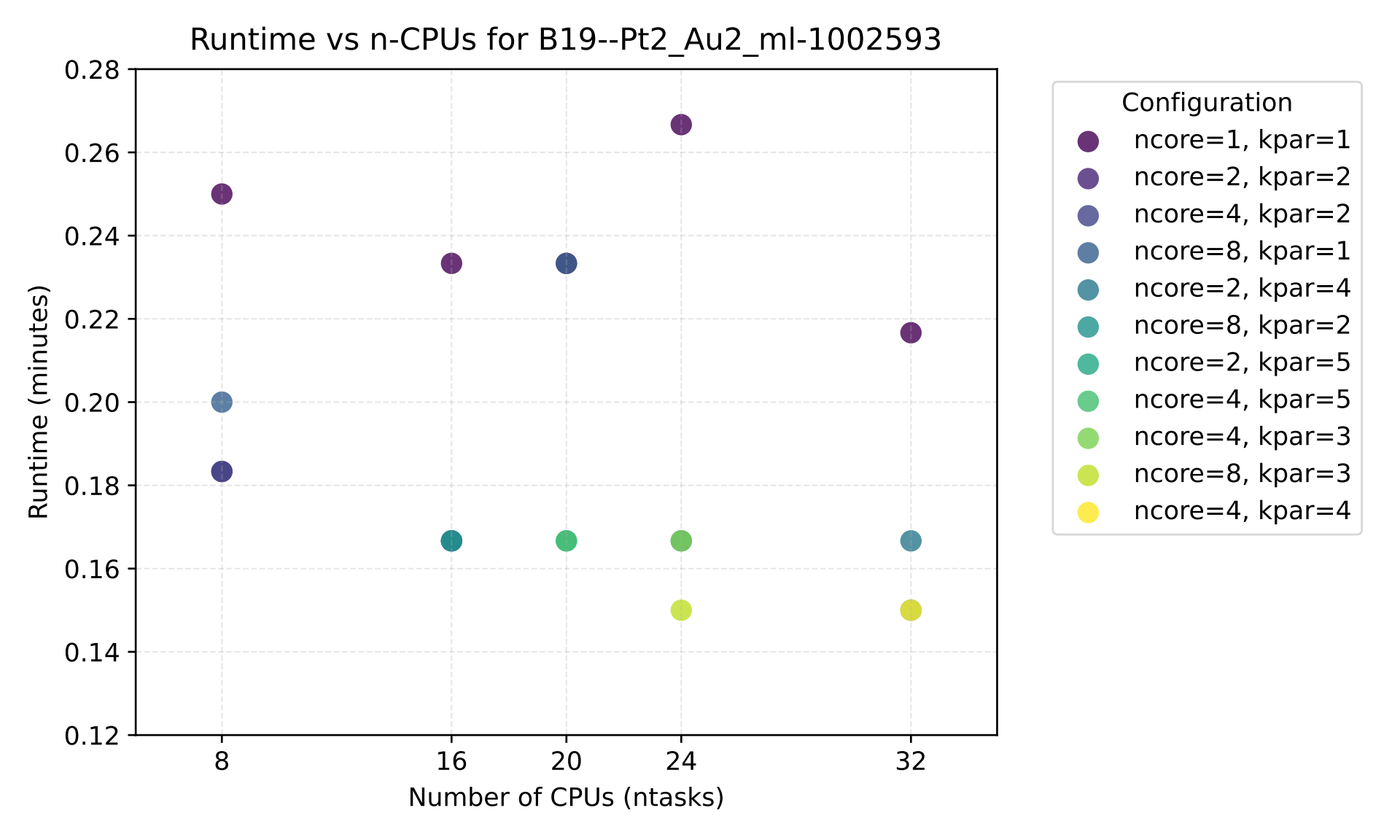
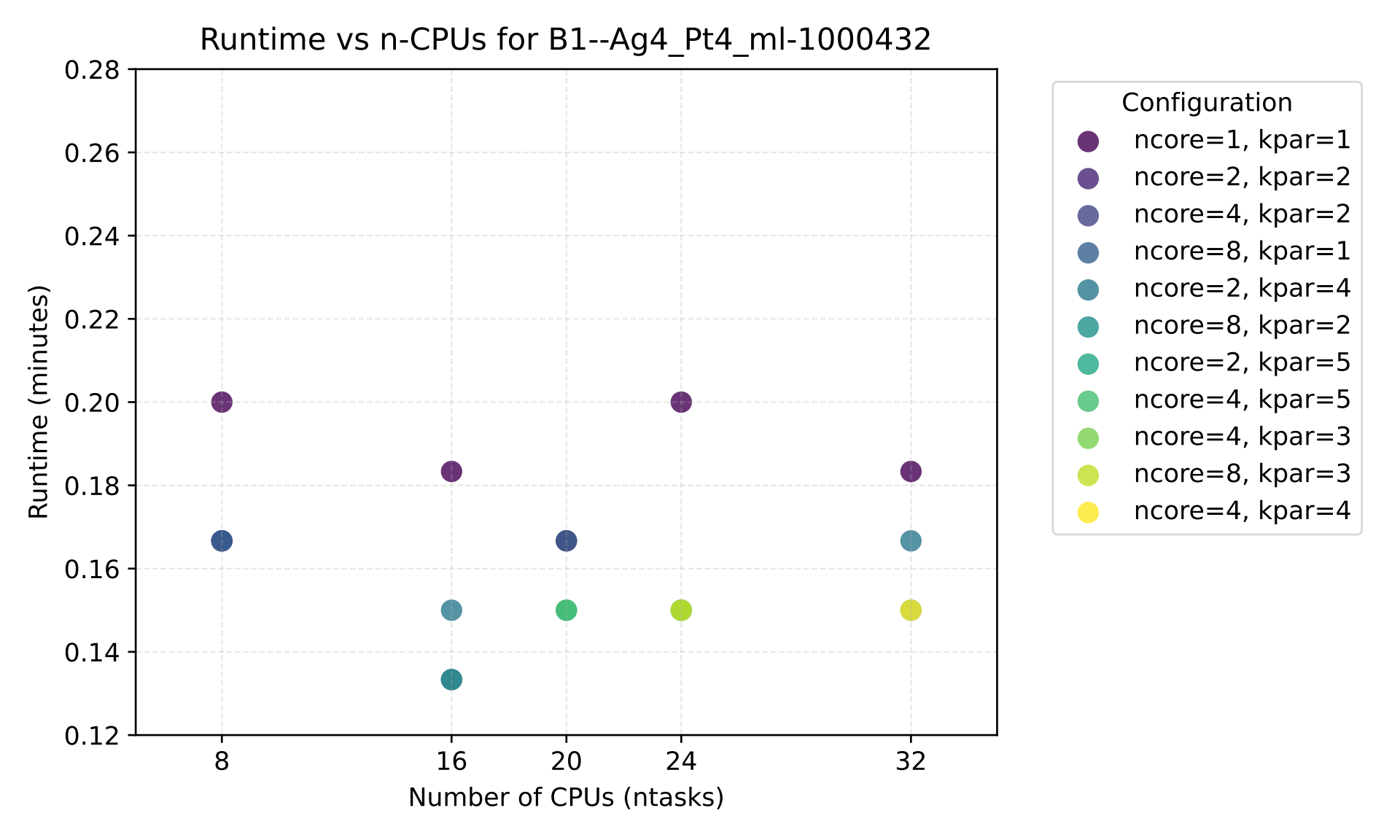

Runtime vs n-CPUs for all Structures
Runtime (minutes)
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
8
16
20
24
32
Number of CPUs (ntasks)
Configuration
ncore=1, kpar=1
ncore=2, kpar=2
ncore=4, kpar=2
ncore=8, kpar=1
ncore=2, kpar=4
ncore=8, kpar=2
ncore=2, kpar=5
ncore=4, kpar=5
ncore=4, kpar=3
ncore=8, kpar=3
ncore=4, kpar=4


Runtime vs n-CPUs for B11--Hf2_Pt2_ml-1002077
Runtime (minutes)
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
8
16
20
24
32
Number of CPUs (ntasks)
Configuration
ncore=1, kpar=1
ncore=2, kpar=2
ncore=4, kpar=2
ncore=8, kpar=1
ncore=2, kpar=4
ncore=8, kpar=2
ncore=2, kpar=5
ncore=4, kpar=5
ncore=4, kpar=3
ncore=8, kpar=3
ncore=4, kpar=4


Runtime vs n-CPUs for B19--Pt2_Au2_ml-1002593
Runtime (minutes)
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
8
16
20
24
32
Number of CPUs (ntasks)
Configuration
ncore=1, kpar=1
ncore=2, kpar=2
ncore=4, kpar=2
ncore=8, kpar=1
ncore=2, kpar=4
ncore=8, kpar=2
ncore=2, kpar=5
ncore=4, kpar=5
ncore=4, kpar=3
ncore=8, kpar=3
ncore=4, kpar=4


Runtime vs n-CPUs for B1--Ag4_Pt4_ml-1000432
Runtime (minutes)
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
8
16
20
24
32
Number of CPUs (ntasks)
Configuration
ncore=1, kpar=1
ncore=2, kpar=2
ncore=4, kpar=2
ncore=8, kpar=1
ncore=2, kpar=4
ncore=8, kpar=2
ncore=2, kpar=5
ncore=4, kpar=5
ncore=4, kpar=3
ncore=8, kpar=3
ncore=4, kpar=4