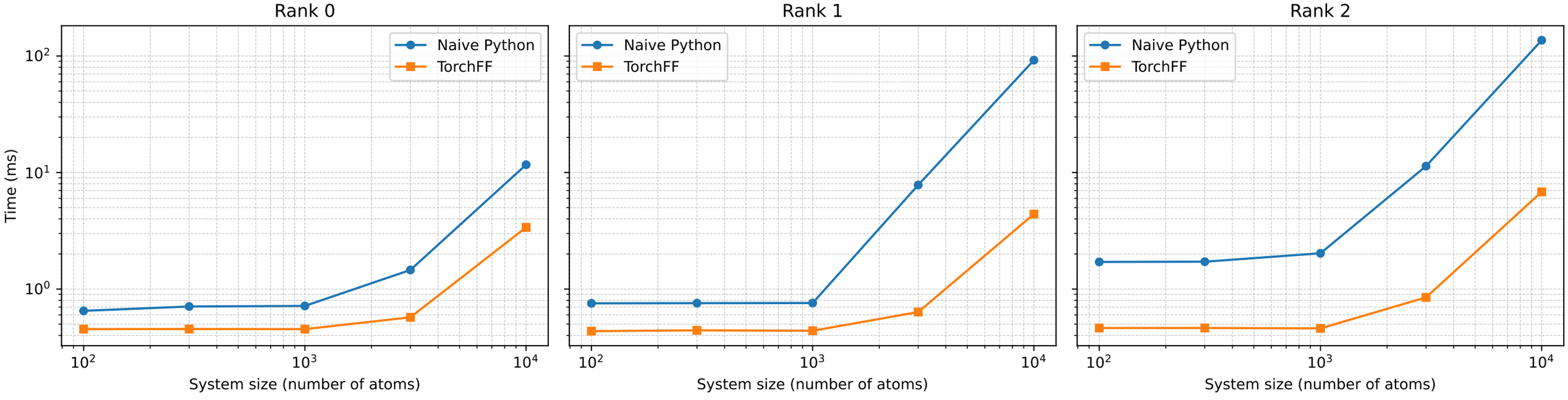
Rank 0
Rank 1
Rank 2
Naive Python
TorchFF
Time (ms)
10^2
10^1
10^0
10^2
10^3
10^4
System size (number of atoms)