NWChem FMC, Add OpenMP to HotSpots (OpenMP #1)

Running Times (s)

Lower is Better

Legend: Pure MPI, OMP=1, OMP=2, OMP=3, OMP=4

X-axis categories: erintsp, ssssm, destbul, obasai, trac12, xwpq, assem, prea4n, wt2wt1, amshf, Total

Y-axis: 1, 10, 100
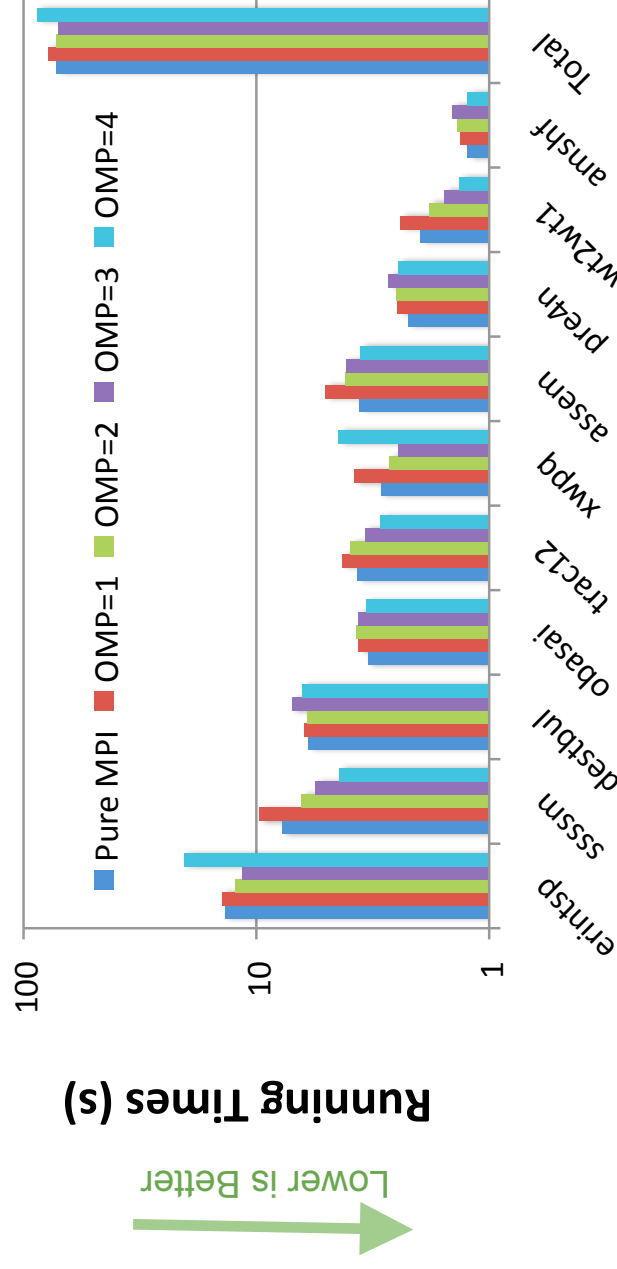
- Total number of MPI ranks=60; OMP=N means N threads per MPI rank.
- Original code uses a shared global task counter to deal with dynamic load balancing with MPI ranks
- Loop parallelize top 10 routines in TEXAS package (75% of total CPU time) with OpenMP. Has load-imbalance.
- OMP=1 has overhead over pure MPI.
- OMP=2 has overall best performance in many routines.

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB — Lawrence Berkeley National Laboratory

NERSC 40 YEARS at the FOREFRONT