We always have 1 OpenMP thread per thread-MPI rank by default. This is best at small/medium rank and simple. But with 128 core nodes, this might no longer be the best. It might even limit the system size when we will soon communicate the whole tpr as one chunk of memory.

Bump

Tested 140k membrane protein system with H-bond constraints on Skylake with 96 threads and 96 ranks, 1 thread is fastest.

Berk, can you upload the data for this?