The more frequent we reorder the Slater matrix, the more localized matching we are using.

Test.

With an equilibrium state, we run 2000 MC steps to test three different reordering procedures.

1. We reorder the matrix every 50 accepted moves.
2. We reorder the matrix every 100 accepted moves.
3. We reorder the matrix when the smallest diagonal element becomes smaller than what is now, or when the trace is decreased by at least 1.

This test system is N = 1024, 3D, K = 1. We are using diagonal preconditioned GMRES with tolerance 1e-5.

First, let’s look at the number of iterations and the number of rows we reordered. The average numbers of iterations are 82.26, 80.98, and 78.89. So all three reordering work well.

C:\Downloads\Optimal reordering Monte Carlo Test\new_scaling_and_ilu\Reorder50.eps

C:\Downloads\Optimal reordering Monte Carlo Test\new_scaling_and_ilu\Reorder100.eps

C:\Downloads\Optimal reordering Monte Carlo Test\new_scaling_and_ilu\ReorderRule.eps

Secondly, the condition number of the matrix shows that all three reordering end up with similar condition number.

C:\Downloads\Optimal reordering Monte Carlo Test\new_scaling_and_ilu\ConditionNumber of reordering steps.eps

Finally, it’s the indices of reordered rows. We can see that they are localized around the row that corresponds to the moving particle.

C:\Downloads\Optimalreordering\local10outof100.epsC:\Downloads\Optimal reordering Monte Carlo Test\new_scaling_and_ilu\c.eps

The conclusion is that we could reorder the matrix less frequently and locally. We could pick a smaller domain and find the matching to reorder the matrix. This is of less cost.