Variational determination of the two-particle reduced density matrix on the GPU

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The quantum many-body problem is plagued by the fact that the Hilbert space explodes exponentially with the system size. All the information necessary to characterize a many-body system is present in the two-particle reduced density matrix (2DM). This fact is exploited in variational density matrix optimization. The difficulty is that you may only vary over N-representable 2DM's: every 2DM must be derivable from a wavefunction. A set of necessary conditions on the 2DM are known which can be written as matrix in function of the 2DM that must be positive semidefinite. The minimalization problem can now be rewritten as a semidefinite program, which is a known convex optimalisationproblem with several algorithms available. Despite the reduction in the dimension of the problem, a semidefinite program remains a hard problem. The technique is currently not competitive with other methods such as coupled cluster.

To improve performance, we try to implement this problem on a GPU (Graphics Processing Unit). GPU's are very fast at massive parallel matrix computations but have only very limited memory available and are more difficult to program. In terms of FLOPS, they outperform a CPU easily. In recent years, many algorithms have been implemented on the GPU with sometimes very impressive speedup's.

A general semidefinite solver is difficult to implement on a GPU because of the memory constraints. However, in our case this is not a problem. We can exploit the specific structure of the problem to reduced the amount of memory needed. The first results show a nice speedup over the CPU program.