Polynomial scaling multireference methods

Sandeep Sharma[a]

[a] *University of Colorado, Boulder*
sanshar@gmail.com

All methods that are used to describe static correlation in multireference quantum chemistry scale exponentially with the size of the active space. This means that one has to be extremely stingy in choosing the active space. This, in turn, implies that one cannot do a black box calculation by say including all orbitals in the valence space for a large system. I will demonstrate that this limitation can be lifted if one uses variational Monte Carlo that is both accurate for strong correlation and also scales polynomially with the size of the active space.

Another difficulty with active space methods is that one cannot calculate dynamical correlation by using multireference perturbation theory or multireference configuration interaction if the active space is large. I will show that this limitation can also be lifted by using stochastic methods that do not require any RDMs in the active space.