Recent developments in FCIQMC

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We will outline several developments in full Configuration Interaction Quantum Monte Carlo (FCIQMC) methodology which my group has implemented recently. These include a new non-uniform method to generate excitations, which greatly increases the efficiency of the method (while not comprosiming the accuracy), and a method to compute reduced density matrices in an unbiased fashion from the stochastically sampled wavefunction. Applications of the new methodology to the calculation of properties such as nuclear gradients, dipole moments and polarisabilities will be presented. We will also present results on a 3-band model of a strongly correlated cuprate, as well as new benchmark calculations of the ionisation potentials of 3d transition metal atoms.