

## **Heat-bath Configuration Interaction: A new, efficient approach to selected CI**

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We present our new selected CI algorithm based on an efficient, deterministic exploration of Slater determinant space, which we call Heat-bath Configuration Interaction (HCI). In sharp contrast to all previous selected CI approaches, HCI identifies the most relevant determinants without first generating long lists of candidates, and introduces a screened sum for the evaluation of the Epstein-Nesbet perturbative correction to the variational energy, enabling vast numbers of determinants that make negligible contributions to be skipped. Both of these improvements result in a highly efficient selected CI algorithm, which is especially well-suited to large basis sets. HCI is naturally combined with our recent semistochastic algorithm to evaluate the perturbative correction in a memory efficient way. We present some recent results using HCI, including the calculation of excited states and the use of HCI as an efficient, deterministic active space solver in large MCSCF calculations.