Preconditioners for Nuclear Configuration Interaction Calculations

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One of the practical approaches to solving a nuclear quantum many-body problem is based on constructing a finite dimensional approximation to the Schrödinger operator in a carefully chosen configuration (basis function) space and computing the smallest eigenvalues and the corresponding eigenvectors of the matrix Hamiltonian. This is often known as the configuration interaction (CI) calculation. To obtain physically meaningful results, the configuration space has to be sufficiently large. This results in a very large but sparse Hamiltonian matrix. Iterative methods are often used to compute the desired eigenpairs. If a few (around 10) eigenpairs are needed, one may use the locally optimal block preconditioned conjugate gradient (LOBPCG) algorithm or the Davidson method to solve the problem. However, without a good initial guess or a preconditioner, we found that LOBPCG typically takes longer to converge than a standard Lanczos iteration even if we have an efficient implementation of the sparse matrix-(multi)vector multiplication procedure. In this talk, I will describe how to choose a good starting guess for LOBPCG in the context of nuclear CI calculation, and how one may construct a good preconditioner to accelerate the convergence of LOBPCG. On massively parallel high performance computer, the construction of an efficient preconditioner must take into account not only the number of operations, but also the amount of communication.