Journal of Computational Physics 229 (2010) 8511–8520

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

A comparative study of iterative solutions to linear systems arising in quantum mechanics

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ARTICLE INFO

Article history:
Received 29 March 2010
Received in revised form 25 July 2010
Accepted 27 July 2010
Available online 4 August 2010

Keywords:
Quantum mechanics
Computational chemistry model problem
Complex nonsymmetric matrices
Lanczos biconjugate *A*-orthonormalization methods
Krylov subspace methods

ABSTRACT

This study is mainly focused on iterative solutions with simple diagonal preconditioning to two complex-valued nonsymmetric systems of linear equations arising from a computational chemistry model problem proposed by Sherry Li of NERSC. Numerical experiments show the feasibility of iterative methods to some extent when applied to the problems and reveal the competitiveness of our recently proposed Lanczos biconjugate *A*-orthonormalization methods to other classic and popular iterative methods. By the way, experiment results also indicate that application specific preconditioners may be mandatory and required for accelerating convergence.

1. Introduction

We consider the numerical solution of the coupled equations for the two-dimensional radial functions on a two-dimensional radial grid for solving a three-body problem in quantum mechanics [1]. Given a total energy E, a Hamiltonian H describing the interaction of two electrons with each other and with the nucleus, an initial state $\Psi^0_{k_i}$ of an electron with momentum k_i incident on a ground state hydrogen atom, find two-dimensional radial functions $\psi^L_{l_1 l_2}$ which solve

$$(E - H_{l_1}(r_1) - H_{l_2}(r_2))\psi^L_{l_1 l_2}(r_1, r_2) - \sum_{l'_1, l'_2} \langle l_1 l_2 \| l'_1 l'_2 \rangle_L \psi^L_{l'_1 l'_2}(r_1, r_2) = \chi^L_{l_1 l_2}(r_1, r_2), \tag{1}$$

where r_1 and r_2 are the underlying coordinates, L denotes the total angular momentum quantum number while l_1 and l_2 denote the single-electron angular momentum quantum numbers, $\chi^L_{l_1 l_2}$ are the radial functions from the expansion of $(H - E)\Psi^0_{k_i}(r_1, r_2)$, $\langle l_1 l_2 \| l'_1 l'_2 \rangle_L$ are two-dimensional coupling potentials arising from the electron–electron interaction, and H_l are the one-dimensional, Coulomb radial Hamiltonians. Refer to the excellent paper [1] by Baertschy and Sherry Li for a complete and detailed description of the original problem as well as its significance in scientific applications.

Discretization of Eq. (1) using finite difference to approximate the derivatives results in a large and very ill-conditioned linear system in the following form:

$$Ax = b, \tag{2}$$

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doi:10.1016/j.jcp.2010.07.034

where $A \in \mathbb{C}^{n\times n}$ is a complex-valued non-Hermitian and nonsymmetric matrix, b is a known right-hand side, and x is unknown to be determined.

The already existing two typical and representative complex nonsymmetric linear systems obtained from the above-mentioned problem, denoted as M3D2 and M4D2, are two instances of a computational chemistry model problem listed in the following table (refer to [2]).

M3D2 and M4D2 have recently received intensive attention in the literature. Day and Heroux [2] showed that 2-by-2 block formulations obtained equating the real and imaginary parts of Eq. (2) can help nonsymmetric Krylov subspace methods perform reasonably well with standard incomplete LU (ILU) factorizations, competitively with ILU-preconditioned Krylov methods applied to the original complex system. Motivated in part by these work of Day and Heroux, Benzi and Bertaccini [3] further considered real-valued preconditioned iterative methods for the solution of complex linear systems, with an emphasis on symmetric (non-Hermitian) problems. The present paper is devoted to the development of iterative solutions to such problems. The focus of this paper is on experiments of various iterative methods applied to the above-mentioned problems in both situations of no preconditioning and simple diagonal preconditioning, hopefully to demonstrate the competitiveness of our recently proposed Lanczos biconjugate A-orthonormalization methods [4–6] to other classic and popular iterative methods [7] in the field of molecular dynamics.

In this study we consider the complex formulation (2). For simplicity and convenience of comparison, diagonal preconditioning here means row diagonal scaling of the original coefficient matrix and then applying iterative methods to the diagonally scaled matrix. For other elegant preconditioning techniques to improve the performance and reliability of Krylov subspace methods, refer to the outstanding survey by Benzi [8] and the distinguished book by Saad [9].

The paper is outlined as follows: In Section 2, the Lanczos biconjugate A-orthonormalization methods including the BiCOR, CORS, BiCORSTAB algorithms are briefly introduced. The spectral properties of the involved matrices are investigated in Section 3. The results of numerical experiments, carried out with machine precision 10^{-16} in double precision floating point arithmetic in MATLAB 7.0.4 with a PC-Pentium (R) D CPU 3.00 GHz, 1 GB of RAM, are presented and discussed in Section 4. Finally, conclusions are summarized in Section 5.

2. Lanczos biconjugate *A*-orthonormalization methods for linear systems

In this section, the pseudocodes for the preconditioned BiCOR, CORS and BiCORSTAB methods with a left preconditioner M can be represented by Algorithms 1–3, respectively. It can be observed that one iteration of the unpreconditioned BiCOR method requires one matrix–vector product by A and one by A^H while the unpreconditioned CORS and BiCORSTAB methods both require two matrix–vector products only by A instead of A^H.

With respect to detailed derivations of these three novel methods, see [4]. For the applications of these three latter methods for the solution of dense complex non-Hermitian linear systems arising from the Method of Moments discretization of Maxwell's equations, refer to [5,6].

Note that all the three present algorithms demand a polynomial $P(t)$ in t for the choice of the initial shadow residual vector r_0^*. In practical applications for dealing with realistic problems, the optimal choice of the initial polynomial $P(t)$ is problem dependent and may be found on a trial and error basis. Based on our previous experience, it is stressed that when there is no ambiguity or other clarification, the specific default choice for the initial polynomial $P(t)$ is taken to be t in our numerical experiments.

Algorithm 1 (*Left preconditioned BiCOR method*).

1: Compute $r_0 = b - Ax_0$ for some initial guess x_0.
2: Choose $r_0^* = P(A)r_0$ such that $\langle r_0^*, Ar_0\rangle \neq 0$, where $P(t)$ is a polynomial in t. (For example, $r_0^* = Ar_0$).
3: **for** $j = 1,2,\ldots,$ **do**
4: **solve** $Mz_{j-1} = r_{j-1}$
5: **if** $j = 1$ **then**
6: **solve** $M^H z_0^* = r_0^*$
7: **end if**
8: $\hat{z} = Az_{j-1}$
9: $\rho_{j-1} = \left\langle z_{j-1}^*, \hat{z}\right\rangle$
10: **if** $\rho_{j-1} = 0$, **method fails**
11: **if** $j = 1$ **then**
12: $p_0 = z_0$
13: $p_0^* = z_0^*$
14: $q_0 = \hat{z}$
15: **else**
16: $\beta_{j-2} = \rho_{j-1}/\rho_{j-2}$