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**TITLE: A DIRECT ITERATIVE-VARIATIONAL METHOD FOR SOLVING
LARGE SETS OF LINEAR ALGEBRAIC EQUATIONS**

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A Direct Iterative-Variational Method for Solving
Large Sets of Linear Algebraic Equations

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Abstract

We have developed a direct iterative-variational technique for solving large systems of linear equations: $Ax = b$, where N is the order of the matrix A and the length of the vectors x and b . The method, which has analogues in the conjugate gradient and Lanczos schemes as well as the direct configuration-interaction procedures of quantum chemistry, involves the construction of an orthonormal basis from successive applications of the general linear algebraic (LA) matrix, A , to an initial guess for the solution vector. The solution vector is expanded in this basis, and the coefficients are determined from a variational prescription. For n iterations, the number of operations to solve the LA equations is of the order N^2n . Since the basis is orthonormal, the procedure is guaranteed to converge within N iterations, provided that the basis vectors remain linearly independent. In practice, the convergence is much more rapid ($n \ll N$). Another advantage of the method is that the whole matrix A need not be stored. In the more general case of multiple right-hand-sides (x and b , matrices), the method can be applied simultaneously to all of the solutions, thus saving many redundant operations that would arise from treating each column of x independently.

We have applied the technique to the solution of LA systems that arise from converting radial coupled integrodifferential equations to an integral representation on a discrete quadrature, in particular, to a variety of problems for electron-atom and -molecule collisions. The order of A is given approximately by the product of the number of quadrature points n_p and the number of scattering channels n_c ($N = n_c \times n_p$). Since the method is direct, we need only store the potential, the regular and irregular components of the product Green's function, and the iterates, therefore drastically reducing the central memory requirements. The integrals are constructed from simple recursion relationships involving the stored quantities. In addition, the direct approach results in savings in computational time since the number of operations to generate an iterate scales as $n_c^2 n_p$ rather than N^2 . We generally start the iteration from the Born solution although better guesses such as the distorted wave, may enhance the convergence. As an example, we apply the method to electron collisions with the hydrogen molecular ion at the static level and treat large numbers of coupled channels ($n_c = 30$).

1. Introduction

We describe a general iterative-variational(IV) prescription[1] for solving large sets of linear algebraic(LA) equations. The method has close analogues in the procedures of Lanczos[2], in direct configuration interaction(CI) approaches of quantum chemistry[3-7], and in other iterative-variational schemes[8-9] such as the multilevel adaptive technique[10] based on grid refinement. Since we have described the application of the method to several physical situations, such as electron-molecule scattering, in another set of papers[11-13], we concentrate on the mechanics of the basic method, demonstrating its efficacy on a particular test case.

2. Mathematical Formulation

We divide this section into two parts. In the first part, we present a basic outline of the iterative-variation prescription for a general system of linear algebraic equations. We then in the second part apply the technique to a class of atomic and molecular scattering problems, which involve the solutions of large sets of coupled integrodifferential equations.

2.1 General Prescription

We seek a solution of the following linear system of equations:

$$A x = b \quad , \quad (1)$$

where the order of the matrix $\mathbf{A}$ or the length of the vector $\mathbf{x}(b)$ is N . We view such matrix operations in terms of an N -dimensional linear vector space[14]. We employ bold-face characters to represent the denizens of this space with capitals for matrices and lower-case for vectors. The juxtaposition of two such symbols always implies matrix or vector multiplication. At the heart of our approach lies the basic property that any vector $\mathbf{x}$ can be expanded in terms of a set of orthonormal basis functions $\{\mathbf{x}_i | i=1, N\}$ that span this space:

$$\mathbf{x} = \sum_{i=1}^N a_i \mathbf{x}_i \quad (2)$$

such that $\tilde{\mathbf{x}}_i \mathbf{x}_j = \delta_{ij}$ with the superscript tilde($\sim$) representing a matrix or vector transpose. Therefore, the principal task of the iterative-variation scheme is to generate this basis and the corresponding expansion coefficients in eq.(2).

We construct the orthonormal basis by successive applications of the matrix $\mathbf{A}$ to an initial guess of the solution. In doing so, we take advantage of the property of such N -dimensional spaces that the application of $\mathbf{A}$ to a vector yields a new vector also in this space. In general, this new set of vectors is not orthonormal. We therefore invoke a standard technique, such as the Gram-Schmidt[15], at each iteration to assure orthogonal vectors. We start the iteration with a guess $\mathbf{x}_1$ and define an intermediate vector $\mathbf{y}_1 (= \mathbf{x}_1)$, which for the first step is redundant but at later stages will prove useful. We then construct a normalized vector by

$$\mathbf{z}_1 = n_1 \mathbf{y}_1 \quad (3)$$

where $n_1 = (\tilde{\mathbf{y}}_1 \mathbf{y}_1)^{-1/2}$. We generate the next iterate by applying $\mathbf{A}$ to this vector .

$$\mathbf{x}_2 = \mathbf{A} \mathbf{z}_1 \quad (4a)$$

and employ the Gram-Schmidt procedure to guarantee orthogonality as

$$y_2 = x_2 - O_{21}z_1, \quad (4b)$$

where $O_{ij} = \bar{z}_i \cdot x_j$. We again construct a normalized component by the prescription

$$z_2 = n_2 y_2 \quad (4c)$$

Therefore, for a general iteration m , we have

$$x_m = A z_{m-1}, \quad (5a)$$

$$y_m = x_m - \sum_{i=1}^{m-1} O_{im} z_i, \text{ and} \quad (5b)$$

$$z_m = n_m y_m \quad (5c)$$

In this manner, we produce a basis of m orthonormal vectors $\{z_i | i=1..m\}$.

Once we have a set of such vectors, we must find the expansion coefficients in eq.(2). We choose a variational prescription to effect this result. Several procedures lead to the final form so that we choose to illustrate the variational part with a least-squares technique[16]. We assume that an approximate or trial solution is given in terms of m of the iterate vectors ($m \leq N$) as

$$x_t^{(m)} = \sum_{i=1}^m a_i z_i \quad (6)$$

We append the superscript m to the trial vector to indicate its value at a particular iteration. We define an error array, which indicates the departure of the trial solution from the exact result ($\epsilon = 0$), by

$$\epsilon^{(m)} = A x_t^{(m)} - b, \quad (7)$$

and choose the coefficients subject to the condition that they minimize the square error $\epsilon^2 = \bar{\epsilon} \epsilon$, namely

$$\frac{\partial \epsilon^2}{\partial a_i} = 0, \text{ for all } a_i.$$

This condition that the square error be a minimum is met provided that the coefficients satisfy the following set of LA equations[16]:

$$\sum_{j=1}^m M_{ij} a_j = b_i, \quad (8a)$$

where we have

$$M_{ij} = \bar{z}_i A z_j = z_i x_{j+1}, \text{ and} \quad (8b)$$

$$b_i = \bar{z}_i b. \quad (8c)$$

Therefore, to extract the expansion coefficients, we must solve a linear system of equations of the order $m \leq N$. Clearly, if we have to generate all N vectors of this space, we have gained nothing by the iterative prescription since the order of M will then equal that of the original matrix A . For the method to be successful, we must have m much less than N .

An important question remains: what criteria are used to determine a converged solution? We have studied several different schemes in order to

find the most general answer. First and simplest, we compare the difference between two successive trial solutions. In other words, we define a new vector Δ by

$$\Delta = |x_t^{(m)} - x_t^{(m-1)}|,$$

where the trial vectors are given by eq.(6). This quantity gives an error for each element; we find this information rather excessive. In order to concentrate the findings into a manageable form, we usually define either a maximum error, being the largest component of Δ , or an average error, having the form

$$\bar{\Delta} = \sum_{i=1}^N \Delta_i / N,$$

where Δ_i is an element of Δ . We could also employ a root-mean-square error in a similar fashion. Another prescription involves the evaluation of the error array defined by eq.(7). Again, we can use either a maximum or averaged error. Except for the very small solution elements, which are usually not important in determining actual physical quantities such as cross sections, we find that the average error gives a very good gauge of the convergence. Whatever technique is selected, we define the convergence with respect to a prescribed tolerance, r . If this average difference is within this tolerance, then we stop the procedure; if not, we continue until this condition is reached. Actual tolerances depend on the case under investigation. However, we have found the range 10^{-7} - 10^{-9} to be reasonable for the applications discussed here.

Before leaving this section, we should make several clarifying statements concerning the various steps. First, the iterative prescription is guaranteed to converge in N iterations provided that the linear independence of the iterate vectors is maintained. This claim follows immediately from the fact

that the scheme produces a set of N orthonormal vectors, which span the space. Second, since the prescription involves the multiplication of a known matrix and vector, the whole matrix, A , need not be stored in central memory, resulting in a drastic savings in storage. In the next section, we derive a direct technique for generating the desired iterates for a particular class of scattering problems in order to foster further savings of storage and time. Third, since each basis functions, z_i , is produced by a matrix-vector multiplication, the computational time for m iterations goes roughly as mN^2 rather than N^3 as in most factorization prescriptions. As long as m is much less than N , we achieve substantial savings. Fourth, the order of the small LA equations(8a) that must be solved for the coefficients, a_i , is m and, in most cases considered, relatively small. This set is usually solved by a standard LU factorization method since the storage requirements are minimal. Fifth, the initial guess usually involves a compromise between accuracy and complexity. The better this guess, the more rapidly the iterative procedure is likely to converge. On the other hand, more accurate initial solutions require a greater investment of effort and computational time. A practical balance must be struck for each situation. Sixth, the convergence by iteration need not be uniform. In fact, during early stages of the iterative process, we sometimes observe oscillations in the average error as a function of iteration. Once a reasonable guess to the solution is found, the convergence is usually swift and monotonic in the error. Seventh, we occasionally encounter linear dependency in the basis. We base our criterion for removing the offending vectors on the eigenvalues of the overlap matrix. With these considerations, we are ready to address an actual physical problem.

2.2 Applications: Atomic and Molecular Scattering

We can cast many of the scattering problems in atomic and molecular physics in terms of a set of coupled, radial differential equations of the form:

$$L \phi(r) - V(r) \phi(r) = 0, \quad (9)$$

where

$$[L]_{\alpha\beta} = \left(\frac{d^2}{dr^2} - \ell_\alpha(\ell_\alpha + 1) r^{-2} + k_\alpha^2 \right) \delta_{\alpha\beta}, \quad (10a)$$

$$[\psi(r)]_{\alpha\alpha_0} = \psi_{\alpha\alpha_0}(r), \quad (10b)$$

and

$$[V(r)]_{\alpha\beta} = V_{\alpha\beta}(r) \quad (10c)$$

The term $\psi_{\alpha\alpha_0}(r)$ represents the radial scattering wavefunction in a given channel α with angular momentum quantum number ℓ_α and energy in Rydbergs of k_α^2 for a particular linearly independent solution α_0 . From the asymptotic behavior of this solution, we extract the reactance or scattering matrix and hence the cross sections for the process under consideration. We have implicitly invoked the close-coupling(CC) approximation in truncating the expansion in terms of channels at a finite number, n_c , leading to a matrix equation of the channel order. We have designated a specific channel by a lower-case Greek letter $[\beta = (s_\beta \ell_\beta)]$, and except for an associated orbital angular momentum ℓ_β , we have left its definition fairly open so that our formulation is the most general possible. For example, in electron-molecule scattering, the quantum number s_β could represent an electronic, vibrational, or rotational state of the target system. In many cases, the "potential" V in eq.(9) is nonlocal, representing such effects as exchange and correlation. However, the nonlocal form only complicates the internal construction of the LA matrices but does not change their dimensionality or basic structure[17]. Therefore, we confine our development to a local potential without any loss of generality in the nature of the iterative-variational scheme.

We convert this set to coupled integral equations of the form[17]:

$$\psi(r) = \psi^0(r) + \int G(r|r') V(r') \psi(r') dr' \quad (11)$$

where the homogeneous solution ψ^0 satisfies

$$L \psi^0(r) = 0 ,$$

and the Green's function

$$L G(r|r') = \delta(r - r') 1_c ,$$

with 1_c the $n_c \times n_c$ unit matrix with respect to channels. We assume that the Green's function is separable, although this is not essential for the basic LA formulation, as

$$G(r|r') = \begin{cases} G^1(r) G^2(r') & r \leq r' \\ G^1(r') G^2(r) & r > r' \end{cases} , \quad (12)$$

where the $G^Y(r)$ components are diagonal matrices with 1 representing the regular component at $r = 0$ and 2 the irregular.

In order to obtain the LA form, we introduce a quadrature of n_p points for the integral in Eq.(11) and evaluate the functions on this discrete mesh -

$$\psi(i) = \psi^0(i) + \sum_{j=1}^{n_p} G(i|j) V(j) \psi(j) w_j , \quad (13)$$

where w_j is a quadrature weight associated with the j -th radial point, r_j .

We represent this set of equations in supermatrix form as

$$\psi = \psi^0 + W \psi , \quad (13)$$

where

$$[\psi]_i = \psi(i) \quad , \text{ and} \quad (14a)$$

$$[W]_{ij} = G(i|j) V(j) \omega_j \quad . \quad (14b)$$

The matrices ψ and ψ^0 have a size of $N \times n_c$ while W is of order N , where $N = n_c \times n_p$. In other words, the solution matrix has the explicit representation

$$\psi = \begin{bmatrix} \psi(1) \\ \psi(2) \\ . \\ . \\ . \\ \psi(n_p) \end{bmatrix} ,$$

where $\psi(j)$ is given by eq.(10b) and is an $n_c \times n_c$ matrix labeled by channels and independent solutions at point r_j . A more convenient method for labeling the supermatrices involves grouping all the points for a given channel. In this case, we have

$$[\psi]_{q\alpha_0} = \psi_{\alpha\alpha_0}(j)$$

with $q = n_p(\alpha-1) + j$ and $\alpha = 1 \dots n_c$. The blocks of W are now $n_p \times n_p$ matrices labeled by two channel indices (α, β) . The matrix W is usually not symmetric nor diagonally dominant for scattering cases. At this juncture, we

could simply make the indentifications:

$$\begin{aligned} \mathbf{A} &= \mathbf{1} - \mathbf{W} \\ \mathbf{b} &= [\psi^0]_{\alpha_0} , \\ \mathbf{x} &= [\psi]_{\alpha_0} . \end{aligned} \tag{15}$$

and continue with the iterative-variational scheme, applied to each linearly independent solution α_0 , as outlined in section 2.1.

We find, however, that the iterative prescription proceeds in a more stable fashion if we generate the iterates from $\mathbf{W}$ rather than $\mathbf{A}$ and if we employ the quadrature weights in the construction of the inner products. In other words, the procedure, described by eqs.(3)-(5), for generating the orthonormal basis is followed except that the $\mathbf{x}$ vectors are developed as

$$\mathbf{x}_m = \mathbf{W} \mathbf{z}_{m-1} ,$$

rather than by eq.(5a), and the inner product is defined as

$$\langle \psi | \psi \rangle = \sum_{\beta, j} \psi_{\beta \alpha_0}(j) \psi_{\beta \alpha_0}(j) w_j .$$

The error matrix and $\mathbf{a}$ -coefficients are still determined from $\mathbf{A}$ as prescribed in eqs.(6)-(8). As we remarked before[1], successive applications of $\mathbf{W}$ to the homogeneous solution may be viewed as a perturbation or Born series expansion. With these changes, the scheme proceeds as in the previous section.

We now cast the method in a direct form in which the iterates are constructed without creation of the full matrix $\mathbf{W}$. This approach, which has been effectively utilized in CI calculations, results in large savings of storage and to some extent computational time. By using the implicit radial

dichotomy inherent in the separable Green's function, we rewrite eq.(11) as

$$\psi(i) = \psi^0(i) + G^1(i) I^2(i+1) + G^2(i) I^1(i) , \quad (16)$$

where

$$I^1(i) = \sum_{j=1}^i G^1(j) V(j) \psi(j) w_j , \quad (17a)$$

and

$$I^2(i) = \sum_{j=i+1}^{n_p} G^2(j) V(j) \psi(j) w_j . \quad (17b)$$

This formulation leads quite naturally to recursion relations for these quantities:

$$I^1(i+1) = I^1(i) + Q^1(i+1) , \quad (18a)$$

and

$$I^2(i-1) = I^2(i) + Q^2(i-1) , \quad (18b)$$

where $Q^1(i) = G^1(i) V(i) \psi(i) w_i$. We recur upwards on the regular component and downwards on the irregular one, which is the most stable prescription. We observe that to construct the iterates, we no longer have to store the full matrix but only the components of the Green's function, the potential, and the iterate vectors. This greatly reduces the amount of storage required and makes the procedure practical even on computers with relatively small amounts of central memory. In addition, we save some computational time since the generation of each iterate for the direct process scales as approximately n_c^2 rather than $(n_c n_p)^2$ as for the matrix-vector multiply case [eq.(15)].

However, we rarely gain the full advantage of this difference since the latter process is more amenable to vector optimization than the former. One final point is in order. The form of eq.(16) closely resembles that of the integral-equations propagation techniques pioneered by Sams and Kouri[1].

The principal difference rests in the operations performed on the solution vector. For the iterative scheme, we operate on a known vector. Therefore, we can use the most stable directions in the recursion formulae. However, in the propagation scheme, the solution vector must always be determined at the next outward step, thus allowing only forward recursion. Certain stabilization prescriptions must then be invoked to guarantee linearly independent solutions. Such techniques are not required in the IV approach.

In the above derivations, we have applied the IV method to one linearly-independent solution at a time. We find a more efficient prescription results from performing operations simultaneously on all independent solutions. While requiring more storage, the number of redundant calculations is reduced, resulting in a gain of speed. For example, we now start the iterative prescription using all n_c initial vectors and define a matrix X_1 containing these solutions as columns. We then apply W to X_1 and obtain a new set of n_c vectors as

$$X_2 = W X_1 \quad (19)$$

We follow the usual procedure and construct a set of orthonormal vectors. We then use these $2n_c$ linearly-independent vectors to define a basis for the new trial solution. Application of the variational scheme mixes the components of the various solutions usually providing a more rapid convergence. The scheme is continued as before until convergence is reached, except that now we generate n_c new vectors at each iteration or cycle.

3. Numerical Calculations

The applications to several physical problems in electron-molecule and -atom collisions have been given elsewhere[1,11-13] so that we shall concentrate on the actual computational procedures. As a specific test case, we apply the method to electron-impact excitation of the hydrogen molecular ion H_2^+ in the static approximation in which exchange and correlation effects are neglected. In addition, we "freeze" the nuclei in a fixed position throughout the scattering event so that rotational and vibrational motion is not allowed. Therefore, we consider only the electronic excitation of the target molecule. The electronic states of H_2^+ are generated from standard molecular structure programs using an 80-function primitive Gaussian basis. This basis provides an accurate representation of the target as demonstrated by the excellent agreement between the calculated state energies and the exact results[19]. We also make a single-center expansion of the system and target wavefunctions about the center-of-mass of the molecule. Each channel, α , is labeled by a particular electronic state s and an associated angular momentum l_s . We let n_s be the number of states and n_l the number of orbital angular momenta in each state so that the total number of channels becomes $n_c = n_s \times n_l$. We consider a radial mesh divided into five subregions as:

$$(0., 1.); (1., 2.); (3., 6.); (6., 10.); (10., r_a)$$

where r_a is $15a_0$. For each subregion i , we choose a number of points n_p^i and distribute them according to a Gauss-Legendre quadrature scheme. The total number of points n_p equals the sum of all subregions. The order of the 1A equation that must be solved is $N = n_c \times n_p$. In Table 1, we present the results for several different meshes for the three-state case, $(1\sigma_g, 1\sigma_u, 2\sigma_g)$.

For the first three IV entries, we vary the size, N , of the LA system by changing the number of points in the radial mesh. For the 50, 100, and 180 point cases, we employ distributions of (10,20,10,10,10), (20,40,20,10,10), and (40,60,40,20,20) respectively. The actual number of points in the calculations is always one greater since in the LA prescription we include a zero-weight point at r_a . All IV calculations reported in the Table were performed by the direct prescription with the initial guess confined to the homogeneous solution ψ^0 . In the case of electron-ion scattering, this homogeneous term is simply composed of regular Coulomb functions. For completeness, we compare the IV results with a standard LU factorization routine, SGECON/SGESL, from the LINPACK library[20], which has been optimized for vector processing[21]. All times refer to CPU on a CRAY I. We observe that the first three entries scale linearly in n_p as predicted from our derivation of the direct procedure. For the smallest matrix system, the LU and IV methods are comparable in time. This at first may seem contradictory since only nine iterations were required for each linearly independent solution. The resolution of this conundrum comes from the highly optimized vector routines used to evaluate eq.(15). The IV procedure by contrast cannot be as significantly optimized. However, by the next larger case, the method has greatly outstripped the LU approach. One other point should be made, we have not included the time to create the W matrix in t_{LU} . By comparing the third and fourth entries, we observe about a twenty percent savings resulting from treating all linearly independent solutions together. This savings should become more pronounced for larger systems. Finally, we present a case for a matrix of order 3000. The timings are very competitive with other iterative procedures[10]

4. Conclusions

We have described the basic mechanics behind an efficient and highly effective direct iterative-variational scheme for solving large systems of linear algebraic equations. The method has two distinct parts. In the iterative part, we construct a set of orthonormal vectors by successive applications of the matrix to an initial guess for the solution. The variational step consists of applying a least-squares technique to finding the optimum expansion coefficients of this basis to represent a trial solution vector. If the number of iterations, and therefore the number of basis vectors, is small compared to the order of the matrix, the method has distinct advantages over standard LU factorization approaches. For scattering problems, the method also lends itself to a direct formulation by which the full matrix need not be generated or stored, thus saving substantial memory and computational time. We find the procedure highly competitive with other direct iterative approaches.

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Table 1

Comparison of computational times for IV and LU factorization techniques for electron scattering from H_2^+ in the 3CC static approximation at 1.7Ry. The nomenclature is as follows: n_c -number of channels, n_p -number of radial mesh points, N -order of the LA system ($=n_c \times n_p$), n_i -number of iterations/independent solution, t -time in CPU seconds on a CRAY I. The symbol Mt represents the method of the IV solution: A for all independent solutions at once, I for a solution at a time. The ratio of the times of the current and initial entries is given by R . All IV calculations are by the direct procedure starting from the homogeneous solution with a tolerance on the rms error of 1×10^{-8} .

n_c	n_p	N	Mt	n_i	t_{IV}	R_{IV}	t_{LU}	R_{LU}
9	61	549	A	9	1.07	1.00	0.90	1.00
9	101	909	A	9	1.66	1.55	4.46	4.96
9	181	1629	A	9	2.83	2.65		
9	181	1629	I	13	3.33	3.11		
30	101	3030	I	40	67.0			