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Using a biconjugate gradient method to solve the electric field - charge density matrix equation obtained in 3-D resistivity integral equation modelling approach

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In 3-D resistivity modelling using the integral equation technique, the electric field - charge density matrix equation can be written in the simplified matrix form of $E = K.Q$, where E is the electric field intensity, Q is the unknown surface electric charge density and K is the coefficient comprising several other parameters or components. To solve these matrix equations, either direct or iterative methods may be used. Although direct methods such as LU decomposition always provide solutions to the matrix equations, they become inefficient when the coefficient matrix is large. Furthermore, direct methods are more likely to be affected by round-off errors. On the contrary, iterative (or indirect) methods for the case of large matrix equations are more economical in computer memory requirements, and also they are self-correcting if an error is made in the process (iterations) leading to the solution. The conjugate gradient (CG) technique, which is one of the most efficient iterative methods available, can be used for this purpose. The CG method has several algorithms. The simplest, called the classical or ordinary conjugate gradient (OCG) algorithm, solves a matrix equation only in the case where the coefficient matrix is symmetric and positive definite. However, the coefficient matrix in the matrix equations we are faced with here is not necessarily symmetric or positive definite. Hence, the biconjugate gradient (BCG) approach is used in a new application for the solution of the electric charge density in 3-D resistivity modelling problem.

Once the elements of E and K matrices are computed using various Green's functions in the integral equation approach, the above matrix equation is solved for Q. This requires us to compute the inverse matrix K, i.e. K^{-1}. In the OCG method, the function minimisation is carried out by generating a succession of search directions and im-

proved minimisers and after N iterations the solution is obtained. However, the BCG method, in general, does not have a simple connection with function minimisation, and since at each iteration no function is minimised, the method is not guaranteed to converge until N iterations. However, the rate of convergence can be quite fast if the eigenvalues are bunched together. Also, by preconditioning of the coefficients matrix (i.e. matrix K here), the rate of convergence may be accelerated. This suggests that applying a preconditioner $\tilde{K}$ to the above equation yields the following equivalent equation system, which is to be solved: $(\tilde{K}^{-1}.K).Q = \tilde{K}^{-1}.E$, where $\tilde{K}^{-1}$ is an approximate inverse of K (i.e. $\tilde{K}$ is close to K) so that $\tilde{K}^{-1}.K \approx 1$. This idea allows the algorithm to converge in fewer steps. In the computer program, developed in this research, we have used the trivial diagonal part of the matrix K as the preconditioner $\tilde{K}$.

The BCG method uses two similar conjugate search direction vectors p_i and $\bar{p}_i$ resulting in two residual vectors ε_i and $\bar{\varepsilon}_i$ (for $i = 1,\ 2,\ ....$). These quantities correspond to the matrix K and its transpose K^T. We supply the initial vectors ε_1 and $\bar{\varepsilon}_1$, and set $p_1 = \varepsilon_1$, $\bar{p}_1 = \bar{\varepsilon}_1$. Then we compute quantities α_1 and β_1 from the equations used in this method. Solving the above matrix equation by the BCG algorithm requires an initial guess Q_1 for the solution. Therefore, the residual ε_1 is obtained as $\varepsilon_1 = E - K.Q_1$. Using the following recurrence scheme, we build up the sequence of improved estimates for Q: $Q_{i+1} = Q_i + \alpha_i.p_i$. This guarantees that the residual ε_{i+1} corresponding to Q_{i+1} in the recurrence is equal to $E - K.Q_{i+1}$. Since $\varepsilon_{m+1} = 0$, Q_{m+1} is the solution to the above matrix equation.