1 PURPOSE

To calculate the least value of a function, $F(x_1,x_2,...,x_n)$ say, of n variables, where n≥2. The user of this subroutine has to provide an initial estimate of the required values of the variables $(x_1,x_2,...,x_n)$ and he has to provide a subroutine (see Section 3) that calculates $F(x_1,x_2,...,x_n)$ and the first derivatives $\partial F/\partial x_i$, i=1,2,...,n, for any $(x_1,x_2,...,x_n)$.

2 ARGUMENT LIST

The single precision version

```
CALL VA06A(N,X,F,G,STEP,ACC,MAXFUN,IPRINT,W)
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The double precision version

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CALL VA06AD(N,X,F,G,STEP,ACC,MAXFUN,IPRINT,W)
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X,G and W are one-dimensional arrays, and the remaining parameters are all real or integer variables. The user must give values to N, X(I) (I=1,2,...,N), STEP, ACC, MAXFUN and IPRINT. The subroutine adjusts X(I) (I=1,2,...,N) but it does not alter the values of N, STEP, ACC, MAXFUN and IPRINT.

N INTEGER variable set to the number of variables of the objective function, and it must not be less than two.

Initially X(I) (I=1,2,...,N) must be set to an estimate of the required vector of the variables. The subroutine adjusts this vector so that, when the subroutine finishes, it contains the best calculated values of the variables.

F REAL (DOUBLE PRECISION in the D version) variable which will contain the least calculated value of $F(x_1,x_2,...,x_n)$, corresponding to the final vector X(I) (I=1,2,...,n).

The lengths of the arrays G and X must be at least N. G is used for first derivatives $\partial F/\partial x_i$, i=1,2,...,N. The subroutine sets the final values of G(I) (I=1,2,...,N) to the components of the gradients of $F(x_1,x_2,...,x_n)$, for the final vector X(I) (I=1,2,...,N).

STEP REAL (DOUBLE PRECISION in the D version) variable set to a positive number, that is the user's recommendation of the initial change to make to $(x_1,x_2,...,x_n)$ in the search for the least value of $F(x_1,x_2,...,x_n)$. About 1 percent or 10 percent of the total expected change in the vector of variables is usually an adequate value for STEP.

ACC REAL (DOUBLE PRECISION in the D version) variable which controls the accuracy of the calculation. The subroutine finishes when a point $(x_1,x_2,...,x_n)$ is found at which the first derivative vector satisfies the inequality

$$\sum_{i=1}^{n} \left(\frac{\partial F}{\partial x_i}\right)^2 \ ACC^2.$$

This criterion does not <u>guarantee</u> that $F(x_1,x_2,...,x_n)$ is close to its least value, but in most cases it is adequate. If the user is doubtful, he should experiment with different initial estimates of the vector $(x_1,x_2,...,x_n)$.

The parameter MAXFUN is an upper bound on the number of calls of CALCFG (see Section 3) that are made by the subroutine. If this bound is attained before the accuracy criterion is satisfied, then the subroutine finishes, and it prints the diagnostic message "VA06A has made MAXFUN calls of CALCFG". Experiments show that frequently the subroutine requires less than max[100, 10*N] calls of CALCFG, but MAXFUN should be set to a greater number, unless the total amount of calculation needs to be limited by a conservative value of MAXFUN.

IPRINT INTEGER variable which controls the amount of printed output from the subroutine. If IPRINT is zero there is no printing, except perhaps the diagnostic message of the last paragraph. Otherwise the best calculated values of $(x_1,x_2,...,x_n)$ and $F(x_1,x_2,...,x_n)$ are printed after every |IPRINT| iterations, and, if IPRINT is positive, the components of the first derivative vector are printed also.

The elements of the array W are used for working space. The length of W must be at least $(2n^2+6n)$. This array is utilised in such a way that, when the execution of VA06A finishes, its first $\frac{1}{2}$n(n+1) elements are estimates of the second derivatives $\partial^2 F/\partial x_i\, \partial x_j$ (i=1,2,...,n; j=i,i+1,...,n), calculated at the point whose components are the final values of X(I) (I=1,2,...,N). Specifically the estimate of $\partial^2 F/\partial x_i\, \partial x_j$, j ≥ i, is the element W({n–$\frac{1}{2}$i}{i-1}+j). Moreover the next $\frac{1}{2}$n(n+1) locations of W contain the elements of the upper triangle of the inverse of the matrix of the second derivative approximation.

3 SUBROUTINE CALCFG

The subroutine, provided by the user, to calculate $F(x_1,x_2,...,x_n)$ and its gradient, must have the name

SUBROUTINE CALCFG (N,X,F,G)

where N, X, F and G correspond to the N, X, F and G of the parameter list of subroutine VA06A. Subroutine VA06A calls CALCFG once on every iteration, and it assigns the components of X. CALCFG must not change the values of N and X(I) (I=1,2,...,N), but it must set F to the function value $F(x_1,x_2,...,x_n)$, and, for i=1,2,...,n, it must set G(i) to the first derivative $\partial F/\partial x_i$, where $(x_1,x_2,...,x_n)$ is the vector whose components are set in X(I) (I=1,2,...,N).

4 SCALING OF THE VARIABLES

The accuracy criterion, depending on the value of the parameter ACC, is such that it is sensible to scale the variables so that the components of the first derivative vector do not differ much in magnitude. There are other good reasons for trying to achieve this scaling. Differences in scale by factors of up to one hundred are usually not very harmful, but one should certainly try to avoid larger differences, and it is preferable if differences do not exceed the factor ten.

5 THE METHOD OF THE ALGORITHM

The method used is described by M.J.D. Powell in a Harwell report R.6469, 1970, and he gives some properties of the method in a Theoretical Physics Division Report (T.P.393). This method is a hybrid one, based on the steepest descent algorithm and on the generalized Newton iteration. The Newton characteristics provide a fast final rate of convergence to the least value of $F(x_1,x_2,...,x_n)$, and the steepest descent characteristics ensure that, in theory at least, the accuracy criterion will be satisfied. However one cannot expect to meet the accuracy criterion if computer rounding errors can perturb the computed values of $\partial F/\partial x_i$ by amounts that are greater than $ACC/\sqrt{n}$.

6 WARNING

This subroutine assumes that there are no mistakes in subroutine CALCFG. Therefore it is important that the user makes an independent check of his calculation of the derivatives $\partial F/\partial x_i$, i=1,2,...,n.

7 ERROR EXIT

This subroutine may finish because the gradients are wrong, or because computer rounding errors make it impossible to continue the calculation efficiently. In these cases the diagnostic “Error exit from VA06A” is printed. If this diagnostic occurs, and if the final derivative vector does not have small components, then it is probably due to incorrect derivatives.