alloy Zr₂Al₁ which has a face-centered orthorhombic structure and impurity lines in the low-angle region, and the alloy ZrAI which is a mixture of two compounds present in approximately equal amounts, the program is incapable of indexing them directly. The results suggest that the applied indexing method has a certain tolerance to limited impurity lines if there is no serious interference from the systematic absences or dominant zone. However, with the deductive indexing approach, possible impurity lines may be identified by giving their lattice parameters and removed from the data set before attempting the indexing.

The hydrides were indexed by the deductive method using the relation between the host alloy and its hydride (the hydride usually has an expanded cell of the host alloy). The dimensions of a cell slightly larger than the host alloy were entered, and from the indexed results, the lattice parameters or the powder constants Qₓ were adjusted to fit the indices and then refined. Three hydrides were indexed in this way. Another hydride which has a pseudo-tetragonal structure (monoclinic) could not be simply indexed by an expanded cell, but trial-and-error adjusting of the angle between a and b to 90.57° could match the calculated lines to the observed lines, and an Mₓ of as high as 29-4 could be reached by this indexing.

Considering all the indexed results, for a pattern with good data quality, we would say that an accurate value of the de Wolff figure of merit Mₓ of as low as 3-7 without refinement can give a correct indexing, but values lower than this would usually indicate an incorrect indexing. Careful selection of systematic absences and refinement can usually significantly increase Mₓ of such a correct indexing to above 10 if there is no interference of the impurity lines. On the other hand, no indexing with Mₓ over 20 appeared to be incorrect (except for some indexing with geometrical ambiguous cells or unreduced cells containing common factors in the quadratic forms). Mₓ values between 10 and 20 are quite possibly correct, but the results need to be further confirmed by other identifications.

**Program package**

The program is a whole package without segmentation. The various functions and routines are reached by answering 'Y/N' or numbered questions. The full loading of the program requires a core memory of 620 Kbytes. The program can be operated on a VAX 11/780 sort of computer. The source code is available from this School.

The author wishes to thank Dr N. J. Clark for his valuable suggestions and kind encouragement in this work.

**References**


**RESTRAIN:** restrained structure-factor least-squares refinement program for macromolecular structures. By H. Driessen, M. I. J. Haneef, G. W. Harris, B. Howlin,* G. Khan and D. S. Moss, Department of Crystallography, Birkbeck College, Malet Street, London WC1E 7HX, England

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**Abstract**

A complete description of the current version of RESTRAIN, a program primarily for the least-squares refinement of macromolecular structures, is presented. This description annouces the version that will be released to the academic community. The additional features present in this version are described in detail. The program is compared with two other macromolecular refinement programs. Finally information about documentation and availability is presented.

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The advent of cheaper vector processing computers manufactured by suppliers such as Convex, Alliant and Ardent has increased the need for software which can take advantage of vector hardware. **RESTRAIN** was originally developed on a Cray-lS and was optimized for the vector facilities on that machine. It has since run on Convex and Alliant computers where it also takes advantage of the parallel architecture in a multiprocessor environment.

The most widely used program for the refinement of macromolecular structures is **PROLSQ** written by Hendrickson & Konnert (1980). The main differences between **RESTRAIN** and **PROLSQ** are discussed below.

The program is completely general and may be used for any number of reflections in any space group. The program can be used for any size of problem. The number of atoms which may be refined is only limited by the available memory of the computer used. Array sizes are increased by a global change of the relevant variables in the PARAMETER statements.

Future program developments include the incorporation of subroutines to refine the diffuse scattering data as well as the Bragg data. This will enable the entire diffraction pattern to be used, as the diffuse scattering contains information on the correlation of atomic motions not present in the Bragg data alone.

**Structure of the program**

(a) Overview

**RESTRAIN** is a least-squares refinement program principally for use with protein and nucleic acid structures solved by single-crystal diffraction methods. It involves a least-squares algorithm with pseudo-energy restraints applied to the molecular geometry.

The function minimized in **RESTRAIN** is of the form

\[ M = \sum w_i \left( |F_i| - G|F_i| \right)^2 + \sum w_p (\varphi_i - \varphi_p)^2 \]

\[ + \sum w_d (d_{ij} - d_{ij})^2 + \sum w_r d_{ij}^2 \]

\[ + \sum w_b (b_{ij} - b_{ij})^2 + \sum w_v |V|, \]

where \( w_i \) = structure amplitude weighting coefficients, \( |F_i| \) = observed structure amplitudes, \( G \) = scale factor, \( |F_i| \) = calculated structure amplitudes, \( w_p \) = phase weighting coefficients, \( \varphi_p \) = estimated phases (from isomorphous and/or anomalous data), \( \varphi_i \) = calculated phases, \( w_d \) = restrained distance weighting coefficients, \( d_{ij} \) = target interatomic distances, \( d_{ij} \) = calculated interatomic distances, \( w_r \) = weighting coefficients for restrained distances of chiral tetrahedra, \( w_b \) = weighting coefficients for non-bonded interactions, \( b_{ij} \) = observed distances between two non-bonded atoms, \( b_{ij} \) = minimum distances allowed for such atoms, \( w_v \) = weighting coefficients for planarity restraints, and \( |V| \) = determinant of product-moment matrix of a planar group of atoms.

The program algorithm has been described in some detail elsewhere (Haneef, Moss, Stanford & Borkakoti, 1985), so this will not be repeated here, although a few points to note are that, for non-bonded interactions, the function only operates if \( b_{ij} < b_{ij} \) and that chirality restraints are applied as distance restraints along the edges of chiral tetrahedra. Usually the same weights are given to these as to all other distance restraints.

The above equation may be written as a function of three terms, \( M = M_1 + M_2 + M_3 \), \( M_1 \) representing the first term of (1), \( M_2 \) the second and \( M_3 \) the final four terms. \( M_1 \) is the term conventionally found in crystallographic least-squares procedures, \( M_2 \) is a term allowing the use of estimates of phases from isomorphous and/or anomalous data and \( M_3 \) represents pseudo-potential energy terms. This formulation describes the structure of the program, basically one section dealing with the crystallographic least-squares, \( M_1 + M_2 \), and one section dealing with the pseudo-potential energy terms \( M_3 \).

(b) Input requirements

The program requires as input:

1. The orthogonal coordinates of the molecule to be refined in Brookhaven format. The program will order the atoms in this input with respect to the dictionary.

2. A dictionary containing the restraints to be applied and the coefficients for the form factors. The dictionary has been designed so that users may easily modify it to their own needs and the current dictionary will be supplied with the program.

3. The reflection (and phase) data which can be in binary form. This can be just a set of \( H, K, L \) and \( F_{o,\alpha} \) values or none at all, if geometric regularization only is required. The path through the program is determined by the input data provided.

4. A set of steering data describing the unit-cell lengths, angles and space group. The general equivalent positions for the space group are entered in the same format as in *International Tables for Crystallography* (1983) to avoid unnecessary conversion by the user. The number of items in the reflection file and its format are also specified here; extra restraints and occupancies can be specified. A sample set of steering data is provided with the program and fully explained in the write-up.

The function \( M \) in **RESTRAIN** may be minimized with respect to some of the following parameters: (1) overall scale factor; (2) overall atomic displacement parameter; (3) bulk solvent parameters; (4) atomic coordinates; (5) rigid-body parameters; (6) non-crystallographic symmetry operations; (7) individual isotropic thermal parameters; (8) individual anisotropic thermal parameters; (9) group anisotropic thermal parameters (TLS tensors); (10) atomic, group and coupled occupancies.

User friendliness of input/output has been an important criterion in the design of **RESTRAIN**. The inadvertent selection of mutually exclusive refinement options is intercepted at the input stage and warnings are given if the program is apparently being used in an unsuitable way. No preparation programs need to be used. The authors have endeavoured to print sensible error messages on job failure, and to intercept lethal input.

The next sections describe the additional features added to the release version.

1. Rigid-body refinement

In the initial stages of macromolecular refinement, the errors in the current molecular model may preclude the refinement of the positional parameters of individual atoms, even when full advantage is taken of all legitimate geometrical restraints. These errors may arise from an interpretation of an electron density map based on isomorphous
or anomalous phases or they may be due to the use of a homologous protein as an initial model for starting refinement.

In these circumstances, meaningful parameter shifts may only be obtained if low-resolution data are employed in conjunction with rigid-body parameters. Parameter corrections in least squares are not likely to exceed half the high-resolution cutoff employed. Thus if positional errors of 4 Å are to be corrected, a high-resolution cutoff of 8 Å or more may have to be employed. At such a resolution, the data-to-parameter ratio necessitates rigid-body methods where only six parameters are needed per rigid body.

Traditionally rigid-body refinement has been carried out by refining the centroid of the rigid body and three Eulerian angles in order to describe its orientation (Doedens, 1970; Sussman, Holbrook, Church & Kim, 1977). Eulerian angles in crystallography do not usually give an easy insight into the nature of a rotation. It is usually more instructive to describe a rotation in terms of an angle about a single rotation axis.

A new approach to rigid-body refinement is adopted in RESTRAIN. Rigid-body orientations are represented by three parameters which may be simply related to the direction cosines of the rotation axis (l, m, n) and the angle of rotation (θ). These parameters are the components of a unit quaternion. Quaternions have been used before in crystallography to perform four-circle diffractometer calculations (Clegg, 1984) and to carry out least-squares superposition of molecules (Mackay, 1984). When applied to refinement of rigid-body orientation, quaternions lead to very simple expressions compared with those involved in the Eulerian method. The relevant algebra for unit quaternion refinement will be discussed in a separate paper (Moss, Driessen & Khan, 1989).

2. Non-crystallographic symmetry
There are basically two modes in RESTRAIN to deal with non-crystallographic symmetry. Mode 1 is used in the early stages of refinement at low resolution, where the coordinates of one molecule and the transformation necessary to create the second molecule are read in and refined, and mode 2 where the transformation is not refined, leading to averaging of the two molecules. This illustrates the potential for using constrained refinement in conjunction with restrained refinement. This option is useful, for example, in protein crystals disordered solvent makes a significant contribution to the Bragg scattering at low angles. This is allowed for by applying Babinet’s principle (Langridge et al., 1960). Accordingly modified form factors (or scattering cross sections) f’ are used in the structure-factor calculations:

\[ f' = f - (SB1) \exp \left[ -\frac{1}{2}(SB2)q^2 \right] \] (2)

where \( q = 4\pi \sin(\theta) / \lambda \). If this option is used, the parameters SB1 and SB2 are refined by matrix techniques with the scale factor G and the overall temperature factor U and their refined values may be used in subsequent cycles in the same way as U and G. These parameters are highly correlated and well defined values may not exist. They may also allow for a disordered part of a macromolecule which is not included in the model currently being refined.

4. Structure-amplitude weighting
If the structure-factor model perfectly described the diffraction of the macromolecule, the theory of least squares shows that the structure amplitudes should be given weights which are inversely proportional to their variances. However, due to the disorder present in macromolecular crystals, the structure-factor model is always significantly in error. The final values of residuals and R factors usually owe more to errors in the final model than to experimental errors in the diffraction data.

The object of weighting the structure-amplitude terms is to ensure that terms heavily affected by model or experimental errors are down-weighted. Several weighting schemes may be employed. The simplest (SCHEME=1) applies equal weights to all the reflections. For SCHEME=1 the weight is given by \( w_r = WF(1) \). This is the scheme that should initially be employed.

A second scheme (SCHEME=2) is a modified form of one proposed by Rees (1976) and involves the use of the standard deviations of \( |F_{n}| \) which must be supplied on the reflection file. The weights are given by the formula:

\[ w_r = WF(1)(\sin(\theta)/\lambda)^{WF(2)}/[\sigma^2 + WF(4)|F_{n}|^2] \]

The weighting coefficients WF (2) and WF (4) are chosen so that the mean values of \( w_r(|F_{n}| - |F_{n}|)^2 \) are approximately the same (within a factor of two or three). These mean values may be inspected in the table (weighting analysis) supplied in the output where they are displayed in bins dependent on resolution and \( |F_{n}| \).

A third scheme (SCHEME=3) is derived from Neilson (1977) and employs a more sophisticated formula than scheme 2:

\[ w_r = WF(1)/[(\sin(\theta)/\lambda)^{WF(2)} + WF(3) + |F_{n}| + WF(4)|F_{n}|^2]^{1/2} \]

A fourth scheme (SCHEME=4) is derived from Cruickshank (1965) and can be used when experimental standard deviations are not available or not trusted:

\[ w_r = WF(1)(\sin(\theta)/\lambda)^{WF(2)}/[WF(3) + |F_{n}| + WF(4)|F_{n}|^2] \]

In all schemes the coefficients are estimated from inspection of the weighting analysis table. It should be noted that only relative weights are significant. The choice of the absolute value of weighting factors does not influence the course of refinement.

5. Space-group-specific routines
RESTRAIN is completely general and can be used for any space group. However, space-group-specific structure-factor routines are included for three space groups often encountered with protein crystals: (a) P222, and C222, (nos. 17 and 20); (b) P212121, (no. 19); and (c) P412121, (no. 92). The space-group-specific routines can be used to save...
time and thereby achieve a higher turnaround. CPU-time reductions of up to 50% have been obtained using these routines, although all refinement options are not available with some of the routines (Table 1).

### 6. Comparison with other refinement programs

(a) **Positional parameters**

The main problem encountered with the refinement of macromolecular structures is the poor observations-to-parameter ratio owing to the relatively weak diffraction of most protein crystals. This ratio can be improved by increasing the number of observations and/or reducing the number of parameters.

The former can be accomplished by introducing restraints on bond lengths, bond angles and torsion angles, to maintain proper stereochemistry throughout the refinement. This method of distance restraints was first proposed by Waser (1963) and applied to macromolecular structures by Konnert (1976). The refinement program **PROLSQ** by Hendrickson & Konnert (1980) is based on this restrained-parameter approach.

The number of independent parameters can be decreased by constraining certain groups of atoms to a particular local stereochemistry and refining these groups of atoms as rigid bodies. The program **CORELS** (constrained-restrained least squares) (Sussman, 1985) adopts this approach, taking advantage of the intrinsic rigidity of proteins (e.g. phenyl, tyrosyl, prolyl groups) and nucleic acids (e.g. bases, phosphates, riboses) (Sussman, Holbrook, Church & Kim, 1977). Rigid-group constraints (Scheringer, 1963a) as extended to allow for variable rotation axes (Scheringer, 1963b), together with distance restraints (Waser, 1963) to maintain proper stereochemistry between groups, lead to a large increase in the observations-to-parameter ratio.

**RESTRAIN** includes a facility (based on the Levenberg-Marquardt method) for handling the underdetermined case, where there are more parameters to be refined than there are observations (Moss & Morflew, 1982). This is particularly useful in protein structure refinement where high-resolution data may not be available and allows refinement to be carried out even at low resolutions.

**RESTRAIN** incorporates both constrained and restrained refinement procedures. Distance, bond angle, torsion angle and planarity restraints are used to maintain proper stereochemistry and effectively increase the number of observations. The rigid-body facility allows groups of atoms to be refined as stereochemically constrained rigid bodies. Pseudo-energy distance restraints are also used to minimize unacceptable non-bonded contacts. Whenever an atom or group is shifted by refinement so that two non-bonded atoms approach within a distance less than the specified minimum non-bonded contact radius for the atom type, appropriately weighted restraint terms shift the atom or group to alleviate this unfavourable contact. The approach is analogous to applying a repulsive van der Waals potential. The restraint terms are represented by the last four terms of the function $M$ given by (1).

(b) **Mean-square displacement parameters**

Hendrickson & Konnert (1980) assumed a riding model for bond dynamics and applied restraints between isotropic mean-square displacement amplitudes (MSDA) of bonded atoms. This idea was later extended to the refinement of anisotropic displacements (Konnert & Hendrickson, 1986). **PROLSQ** uses special forms of anisotropic displacements, whose orientation is 'chosen to be consistent with certain directions for maximum and minimum displacements' (Yu, Karplus & Hendrickson, 1985). However, when this strategy was evaluated by molecular dynamics it was shown that the riding model might not be valid (Yu, Karplus & Hendrickson, 1985). Therefore, there are no restraints on the MSDA of atoms in **RESTRAIN**, where the anisotropic displacements of relatively rigid groups were modelled by translation, libration and screw-rotation (TLS) tensors whose components were refined, thus effecting a saving on the number of parameters which would be required for a free anisotropic refinement. Individual anisotropic MSDAs of the group atoms may be calculated from the refined TLS tensors.

The program **CORELS** (Sussman, Holbrook, Church & Kim, 1977) has been extended to enable refinement of the TLS parameters of the rigid bodies, with the positional parameters held fixed. This method has been applied to a dodecamer of DNA (Holbrook & Kim, 1984; Holbrook, Dickerson & Kim, 1985). **RESTRAIN** enables positional parameters to be refined at the same time as the TLS parameters, and has been used for TLS refinement of bovine ribonuclease-A at 1.45 Å resolution, using selected side-chain groups as rigid bodies and also treating the whole molecule as a rigid body (Howlin, Moss & Harris, 1989).

However, where diffraction data of unusually high resolution (1.0 Å) are available, **RESTRAIN** may be used to refine individual anisotropic atomic displacements. This has been done in the case of avian pancreatic polypeptide (Glover, Haneef, Pitts, Wood, Moss, Tickle & Blundell, 1983) which diffracts to a resolution of 0.9 Å.

(c) **Occupancy parameters**

Although the refinement of occupancies is common in small-molecule structures and their high correlation with thermal parameters is well known, with proteins this is less routine.

**RESTRAIN** allows the occupancy of an atom or group of atoms to be refined. Occupancies may be uncoupled, or the occupancy of one group may be coupled with that of another group.

Coupled second sites may be most easily created by using extra dictionary entries and by treating them as separate protein chains. Electron density maps can usually suggest
reasonable starting values for the occupancies. It is always important to study the \( u \) values for the atoms in second sites because of the strong correlation between occupancy and \( u \). Too large a \( u \) value with a low occupancy either means that the coordinates have been built in the wrong position, or that the site is not 'real'.

The active-site residue His 119 of bovine ribonuclease-A has been refined as two sites, with occupancies of 0·8 (A site) and 0·2 (B site) (Borkakoti, Moss & Palmer, 1982).

A version of PROLSQ modified by Finzel (1987) has a different approach to the treatment of occupancies. For example, in the 1·26 \( \AA \) refinement of phosphate-free ribonuclease-A (Wlodawer, Svensson, Sjölin & Gilliland, 1988), the occupancies were not refined (Hendrickson, 1985). Initial values for the occupancies of multiple sites 'estimated' from electron density maps were 'adjusted' in such a way that the temperature factors of the two sites were similar (Svensson, Sjölin, Gilliland, Finzel & Wlodawer, 1986). The occupancies for the water molecules were estimated from difference Fourier maps and ranged from 1·0 to 0·3 with \( B \) values in the range of 12–66 \( \AA^2 \) (Wlodawer et al., 1988). The limitations of this approach are apparent when noting that anomalous behaviour (low \( B \) with occupancy of less than 1) is dismissed as an 'artifact of the refinement' (Wlodawer et al., 1988).

Uncoupled group occupancy refinement may be useful for protein–inhibitor complexes, where the inhibitor is not present in stoichiometric amounts. A value suggested by the electron density map is used as a starting occupancy for the atoms in the group (inhibitor molecule) and this value is then refined. Examples of enzyme–inhibitor complexes refined using RESTRAIN include complexes of ribonuclease-A with cytidine-N(3)-oxide 2'-phosphate (Palmer, Moss, Haneef & Borkakoti, 1984), cytidine 2'-phosphate (Howlin, Harris, Moss & Palmer, 1987), 8-oxoguanosine 2'-phosphate (Borkakoti, 1983) and 2'-cytosine-phosphate-5'-guanine (Aguilar, 1988).

7. Test cases

(a) Run times on different computers

RESTRAIN has been written in standard Fortran77 (ANSI X3.9-1978) with the exception of NAMELIST for the steering data. The program has been designed to take advantage of vector processing computers such as the Convex and Cray. The program uses internal sine, cosine and exponential functions in its structure-factor calculations, which substantially speed up the calculation compared with the use of stored look-up tables of these functions. It furthermore contains Cray-specific statements in the structure-factor-calculating subroutines. However, standard statements have been provided for use on other machines.

Owing to the fact that the program has been written in standard Fortran it is relatively easy to implement the program on different computers. Table 2 gives some benchmark results for an isotropic refinement of a protein in C2221 at 2·5 \( \AA \) resolution. The molecule contains 1598 atoms, and 4679 reflections were used. In Table 2, REAL*4 refers to 32-bit floating-point arithmetic which is equivalent to a mantissa of approximately seven decimal digits. While such precision is adequate for most refinements, instability can result in critical cases. REAL*8 is 64-bit arithmetic giving about 15 decimal digits of precision and is the preferred choice for avoiding ill-conditioned arithmetic.

The benchmark results have been obtained on the different machines under varying workloads. The timings given are not exactly comparable, since some machines include system-time spent by the machine for the job. Nevertheless, the figures give a rough indication of the capacities. Note that most of the time spent in the program is taken up by just two subroutines, LSCALC (setting up the least-squares equations) and FDERIV (structure-factor and derivative calculations). Gains may be expected here when vectorization is used.

(b) Local usage

At Birkbeck College this program has been used for refinement of protein and nucleic acid structures using X-ray or neutron diffraction data. It has generally been used in conjunction with model building using an interactive vector graphics facility. The program has been set up so that the input/output interfaces easily with the graphics model building program FRODO (Jones, 1978) and FFT programs. Coordinate files have the standard Brookhaven format. The only limitation in the current version is the order in which the atoms must be present. However, the program contains an ordering subroutine.

Examples of protein structures which have been refined at Birkbeck College using RESTRAIN include avian pancreatic polypeptide (Glover et al., 1983), bovine ribonuclease-A (Borkakoti, Moss, Stanford & Palmer, 1984) and \( \gamma \)-crystallin-II (Summers et al., 1984).

(c) External usage

The innate flexibility of the RESTRAIN program and algorithm has been demonstrated by its use in generating initial main-chain atom positions in protein crystallography by IBM UK (Morffew, 1983).

(d) General usage

Although RESTRAIN has been written primarily for refinement of macromolecular structures, the use of a user-defined dictionary for interatomic and planar restraints and options, which allows the user to specify additional interatomic restraints and planes, means that virtually any structure can be refined by the program. The program at present uses a four-Gaussian expansion of form factors (International Tables for X-ray Crystallography, 1974). Coefficients for this expansion suitable for X-ray or neutron diffraction may be read from the dictionary. The \( 4 \sin \theta / \lambda \) \( ^2 \) term is calculated from the supplied cell dimensions and need not be supplied in the reflection data file.

Documentation

The authors have endeavoured to produce an understandable and comprehensive set of documentation in a structured form which is available from Dr D. S. Moss. The documentation is stored as 50 pages of text.

Availability

The program is available on application to Dr D. S. Moss and will be supplied on magnetic tape; users will need to supply their own magnetic tape. A copy of the current dictionary and a sample set of steering data will also be supplied.
### Table 2. Benchmark results for RESTRAIN on different computers

<table>
<thead>
<tr>
<th>Machine</th>
<th>Version</th>
<th>Precision</th>
<th>C(s)</th>
<th>L(s)</th>
<th>G(s)</th>
<th>in LSCALC and FDERIV (%)</th>
<th>Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cray-1S</td>
<td>Cray specific Vectorization of LSCALC and FDERIV</td>
<td>REAL+4</td>
<td>9-7</td>
<td>n.a.</td>
<td>69-4</td>
<td>77-0</td>
<td>1-00</td>
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<tr>
<td>Cray-1S</td>
<td>Cray specific Vectorization of all routines</td>
<td>REAL+4</td>
<td>n.d.</td>
<td>n.a.</td>
<td>67-0</td>
<td>77-7</td>
<td>0-97</td>
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<tr>
<td>Cray-1S</td>
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<td>REAL+4</td>
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<td>n.a.</td>
<td>394-9</td>
<td>96-0</td>
<td>5-69</td>
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<tr>
<td>Cray-1S</td>
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<td>n.a.</td>
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<td>70-2</td>
<td>0-72</td>
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<tr>
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<td>n.a.</td>
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<td>75-5</td>
<td>0-61</td>
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<tr>
<td>Cray X-MP/28</td>
<td>Standard (modified slightly) Vectorization of all routines</td>
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<td>n.d.</td>
<td>n.a.</td>
<td>38-6</td>
<td>78-3</td>
<td>0-56</td>
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<tr>
<td>VAX 11/750</td>
<td>Optimization</td>
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<td>31-4</td>
<td>14000</td>
<td>n.d.</td>
<td>208</td>
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<tr>
<td>Convex C1</td>
<td>Standard Vectorization of LSCALC and FDERIV</td>
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<td>~302</td>
<td>n.d.</td>
<td>953</td>
<td>n.d.</td>
<td>13-7</td>
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<tr>
<td>Convex C1</td>
<td>Standard Vectorization of all routines</td>
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<td>n.d.</td>
<td>375</td>
<td>77-3</td>
<td>5-4</td>
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<tr>
<td>Alliant 3CE</td>
<td>Vectorization and concurrence of all routines except EXP, COS loops in FDERIV</td>
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<td>n.d.</td>
<td>753</td>
<td>n.d.</td>
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<tr>
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<td>~6</td>
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<td>&lt;74</td>
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<td>0-4</td>
<td>255</td>
<td>n.d.</td>
<td>Not solved</td>
</tr>
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</table>

Notes: n.a. = not applicable; n.d. = not determined; C = compile; L = link; G = go.

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### References
