

Removal of finite deformation using strain trajectories

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Abstract—A technique is described for removing the effects of finite deformation, given the principal values and orientations of strain at a number of points throughout a deformed body.

Using the principal orientations, strain trajectories are constructed for the deformed state. The body is divided into finite elements bounded by these trajectories. Each element is then unstrained without changing its orientation or position. This process creates artificial voids and overlaps, which are minimized by imparting rigid translations and rotations to the elements according to a least squares method.

The result is the pattern of strain trajectories for the undeformed state. It is shown that the trajectories for the deformed and undeformed states may be used as reference coordinates in order to map the change in shape of any body as it passes from the deformed to the undeformed state or vice versa. The technique is tested using models of a folded layer and a shear zone. It is suggested that the technique is versatile enough to allow for errors in original strain data. Although the technique has so far been applied to two-dimensional deformations, a similar method should be usable in three dimensions.

INTRODUCTION

GEOLOGISTS are obtaining more and more data concerning tectonic strain in rocks. In general these data are becoming more precise, as a result of improved methods of measurement. Given a sufficient number and precision of strain measurements, it is in principle possible to compute the original (pre-tectonic) shape of any deformed rock mass. This is of great importance as an aid in determining the relative displacements across orogenic belts (Schwerdtner 1976, 1977) and in distinguishing between large scale tectonic processes of various kinds (e.g. diapirism versus folding by regional compression). On a smaller scale, the possibility of removing strains is an aid to understanding the formation of folds, shear zones and allied structures.

Cloos (1947) was the first to obtain abundant strain data in a small region and the first to attempt unfolding a fold on the basis of such data. Oertel (1974) went further by introducing the practical notion of domains (that is finite elements) within each of which the strain could be assumed to be homogeneous. The original shape of each element could readily be obtained simply by reversing the strain, but problems arose in fitting together the unstrained elements. Schwerdtner (1977) and Cobbold (1977) have pointed out that if the state of strain is heterogeneous and if the strain at each point is removed in a straightforward way, then conditions of continuity are violated and the material develops fictitious holes or regions of overlap. To avoid such violations, one must also apply suitable translations and rigid rotations. What is more, the amount of rotation must vary from point to point. For a continuous material, Cobbold (1977) has derived exact two-dimensional expressions for rotation gradients in terms of strain gradients. Schwerdtner (1977) has shown how translations and rigid rotations are necessary to ensure maximum compatibility between finite elements. Oertel & Ernst (1978) have used

the finite element method to remove the deformation in a multilayered fold. Thus this method, being simple to apply, has enjoyed a certain measure of success. The fitting of elements, however, has been done piecemeal and by hand. This task is both laborious and somewhat subjective. For these reasons, the present paper introduces a fitting technique that is based on a least-squares method: it minimizes the sum of the distances between adjacent elements.

In a radically different approach, based on Ramsay & Graham's (1970) method of integrating shear across shear zones, Hossack (1978) has suggested that length changes can be integrated along finite strain trajectories. Hossack does not justify his method theoretically and he readily admits it is incomplete, yielding no information regarding rigid rotations. Yet the approach is not only interesting, but, as will be shown, it is theoretically sound.

In theory, the exact equations for continuous materials (Cobbold 1977) should yield better results than the finite element methods, which are at best approximate. In practice, however, a number of problems arise in using the exact equations. First, the equations are only valid if the strain values used are true strains and thus compatible amongst themselves; otherwise there is no unique solution for the rotations. But anyone who has measured strains in rocks will know that his measurements are to some extent suspect, due to errors, inadequate strain markers (of ill-known initial shape or of different rheology from the enclosing matrix), or volume changes of unknown magnitude. Furthermore, there is no unique way of interpolating between strain values measured at discrete localities. Thus it is necessary to find a distribution of strains that are mutually compatible and also a best-fit to the measured values. The problem had not yet been solved for the continuous model.

A second disadvantage of the exact equations quoted

by Cobbold (1977) is that they are complex, even in two dimensions. Equivalent equations in three dimensions have also been derived, but they are even more complex. It appears that the complexity results from the choice of Cartesian coordinates as a reference frame. The equations become much more simple if the reference frames are sets of orthogonal curvilinear coordinates parallel to the finite strain trajectories, and this aspect will be discussed in a forthcoming publication. In the present paper, curvilinear coordinates will be used in a non-mathematical way because they simplify some of the techniques adopted.

The problem of local strain incompatibilities resulting from errors in strain measurement can be overcome by the use of finite elements. If any one element is abnormally large or abnormally small in relation to the room available, it simply overlaps its neighbours or leaves gaps. An objective method is required, however, to ensure that the total amount of overlaps and gaps is at a minimum, and this is a powerful reason for adopting a fitting technique such as the one presented in this paper.

SIGNIFICANCE OF STRAIN TRAJECTORIES

Although for the purposes of this paper there is no need to go into mathematical detail, some of the more fundamental concepts of finite strain will be reviewed briefly, because they provide the basis and the justification of what follows.

Hobbs (1971) deserves credit for introducing into structural geology the most comprehensive treatment of finite strain, that by Truesdell & Toupin (1960). These authors describe a deformation with the aid of three separate coordinate frames, one for the deformed state, one for the undeformed state, and one a common frame (Fig. 1). This last is taken to be Cartesian, but the other two need not necessarily be so. The deformation carries the point X in the undeformed state into the point x in the deformed state. It is always possible to express the deformation at any point as the product of three components, a rigid translation, a rigid rotation, and a pure strain. In three dimensions, there is one unique set of three orthogonal vectors (triad) at X which on deformation becomes a similar triad at x . These define the principal orientations at X and at x (Cauchy 1823). Along these directions at x , the longitudinal strains (or stretches) have maximum or minimum values and the shear strains are zero; similarly, at X the reciprocal stretches have maximum or minimum values. These maximum or minimum values are known as principal values.

If we choose for our coordinate frames at X and at x , two sets of orthogonal curvilinear coordinates which are the trajectories of the principal orientations (strain trajectories, for short), then in terms of these coordinates, the components of shear strain at every point vanish, and the only non-zero components are the principal strains (Fig. 1). This is the great advantage of using such coordinate frames. Furthermore, the angle be-

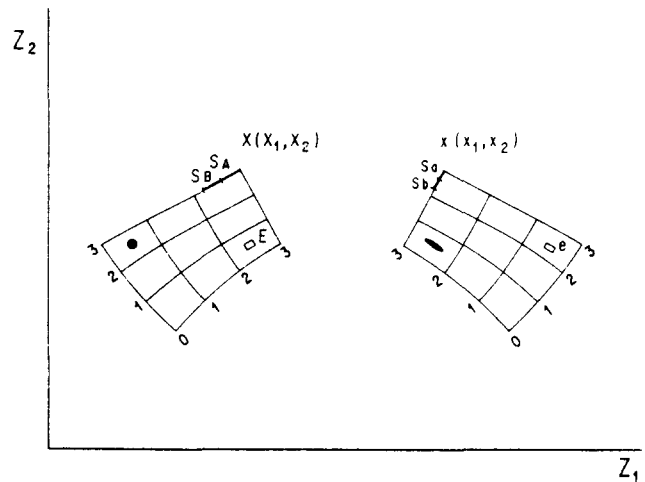


Fig. 1. Coordinate frames for two-dimensional deformation. Common frame (Z) is Cartesian. Frames for undeformed State (X) and deformed state (x) are orthogonal curvilinear and parallel to finite strain trajectories. As a result of deformation, elements of arc S_A and S_B become s_a and s_b , infinitesimal rectangular element E becomes element e , black circle becomes black strain ellipse.

tween corresponding trajectories at X and x is the rigid body rotation (Cauchy 1823).

Now consider two elements of arc, S_A and S_B , lying one next to the other along a strain trajectory at X (Fig. 1). After deformation, the first element has become s_a and it lies along a strain trajectory at x . But S_B has become s_b and it too must lie along a strain trajectory in the deformed state. Therefore unless there is a discontinuity or loss of cohesion between the two elements, both must lie along the same trajectory in the deformed state. By extending this argument it will be clear that the deformation carries the strain trajectories of the undeformed state into the corresponding trajectories in the deformed state. Thus the total length of a trajectory in the undeformed state can be obtained by simple integration of the reciprocal stretch along the corresponding trajectory in the deformed state, and thus the method of Hossack (1978) is fully justified. Indeed, if one were to integrate along all the strain trajectories at the same time, introducing the required rigid rotations, the entire deformation would be removed. The problem with doing this in practice is that it is difficult to take into account any errors in strain values. The finite element method would appear to be more flexible in this respect.

STRAIN TRAJECTORIES AS MAPPING COORDINATES

As with other systems of coordinates, the finite strain trajectories can be used to map the shape changes undergone by any body as it passes from the deformed to the undeformed state, or vice versa. The advantage of strain trajectories over other coordinates is that they are parallel to the principal stretches at all points. Two examples illustrate these points.

Consider first a hypothetical fold (Fig. 2) formed by bending of a layer. In the deformed state (Fig. 2b), the stretches are parallel or normal to the layer boundary and so therefore are the strain trajectories: they form

arcs of circles and radii. In the undeformed state (Fig. 2a), the trajectories are also parallel and normal to the layer boundaries and they form straight lines. This situation is a special one in that the trajectories are Cartesian in the undeformed state. In general they are not necessarily so. It will be clear that the two sets of trajectories can be used to map the shape of the layer boundaries as they pass from the undeformed to the deformed state, or vice versa; the layer boundaries coinciding with one of the coordinate lines in both states.

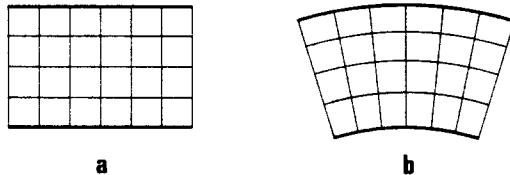


Fig. 2. Hypothetical fold formed by bending of a layer. Strain trajectories in undeformed state (a) are Cartesian; those in deformed state (b) are arcs of circles and radii. Layer boundaries are shown in thick lines.

Now consider a second more complex example, that of a shear zone (Fig. 3). Outside the zone of shear, the rock is undeformed and the strain trajectories have no meaning. If the deformation is considered to be extremely small, however, the trajectories are at 45° and 135° to the shear direction in both the deformed and the undeformed states. Within the zone of shear the trajectories have sigmoidal forms and it can be shown (see, for

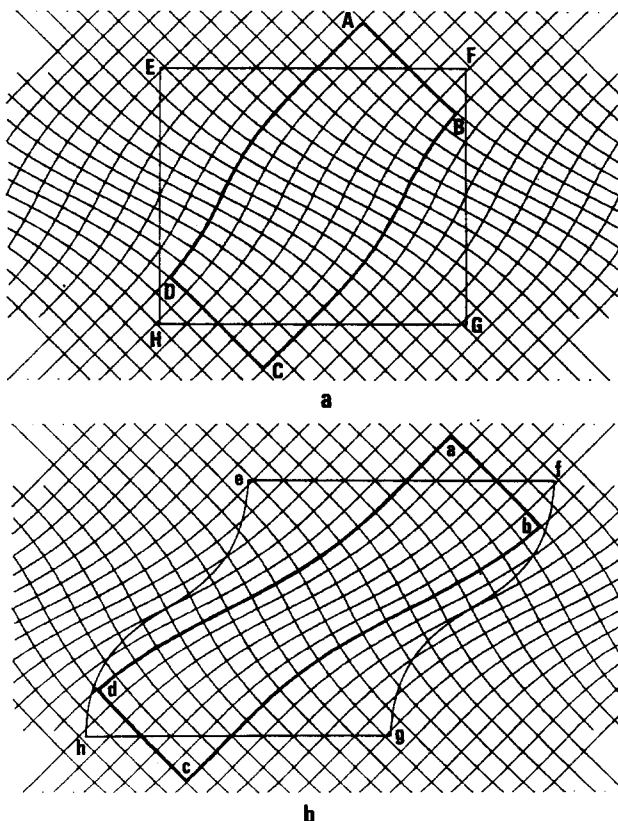


Fig. 3. Hypothetical shear zone. Outside zone of shear, trajectories are Cartesian and orientated at 45° and 135° to shear plane in both undeformed state (a) and deformed state (b). Within shear zone proper, trajectories are sigmoidal. Pattern a is mirror image of pattern b. As a result of deformation, area ABCD becomes area abcd; rectangle EFGH is sheared into form efg, indicating shear strains and displacements across zone.

example, Jaeger & Cook 1969, fig. 17.7) that those in the deformed state (Fig. 3b) are obtained from those in the undeformed state (Fig. 3a) by reflection about a plane of mirror symmetry normal to the shear direction. This symmetry is a special property of simple shear deformations and is not valid for all deformation patterns. If the strain trajectories are used as reference coordinates, the area ABCD becomes the area abcd, and the rectangle EFGH becomes sheared into the shape efg. This last indicates the shear strain across the zone of shear.

These examples of a fold and a shear zone will be used to test the finite element technique introduced in the following section. They also illustrate some of the properties and uses of strain trajectories. Much information can be gleaned from trajectory patterns even if the strain values are not well known. In many rocks, trajectory patterns for the deformed state can be drawn by making the reasonable assumption (Williams 1977) that trajectories are identical to those obtained from the schistosity, the stretching lineation and the normal to both elements. In many other geological examples, principal strain orientations are known with more accuracy than principal strain values. Thus one of the easiest, most reliable and most useful of maps that can be prepared for a deformed region is a strain trajectory map.

FINITE ELEMENT TECHNIQUE

In any finite element technique, the body in question is divided into a finite number of elements of finite size. Assumptions are then made as to the way that all parameters vary within each element. For example, the simplest assumption (that adopted here) is that certain parameters are constant within each element, but vary from element to element. By definition these parameters are therefore discontinuous at element boundaries.

In the technique adopted here, it is assumed that strains, rigid rotations and rigid translations are constant within each element. The problem is to find the translations and rotations in such a way that the elements fit together with a minimum of overlap or voids.

The basic data required for the analysis are: (a) a strain trajectory map or the transformation equations that give the shape of the strain trajectories in space, (b) a map of strain values, or a set of functions giving the variation of strains in space. The strain trajectories can be obtained by fitting curves tangent to the principal orientations as measured at a number of discrete localities. The strain values or strain map can be obtained by a contouring technique or by polynomial approximation. For many two-dimensional problems, graphical fitting of strain trajectories and hand-contouring of strain values are probably sufficiently accurate.

The finite element technique is perhaps best described in stages with reference to examples. The examples chosen here are the fold of Fig. 2 and the shear zone of Fig. 3.

1. The first step is to divide the body into strips of approximately equal width and bounded by the strain trajectories. In two dimensions, this process yields an array of contiguous quadrilateral elements with curved sides that meet at right angles (Figs. 2b and 3b). In three dimensions, the elements are six-sided.
2. The second step is to approximate each element by one which has straight or plane sides. Thus in two dimensions we obtain rectangles and in three dimensions, rectangular prisms. These elements are the ones used for the analysis.
3. The third step is to remove the strain from the elements. The principal strains are parallel to the element sides and the chosen strain values are those of the centroid. Thus the length, breadth and width of the element are simply stretched by the appropriate amounts. The result is another rectangle or rectangular prism, with the same centroid and the same orientation as before (Figs. 4a and 5a).

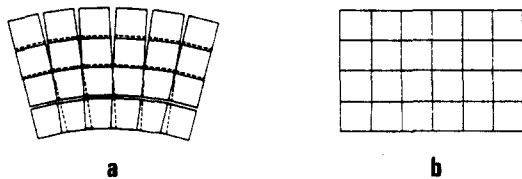


Fig. 4. Unfolding of fold by finite element technique. In first step (a), rectangular elements approximating those of Fig. 2b are unstrained without change of position or orientation, thus creating voids (top) and overlaps (dotted lines). In second step (b), voids and overlaps are minimized, yielding unfolded layer with strain trajectories in undeformed state (compare Fig. 2a)

4. The fourth step is to translate and rotate each element in such a way as to minimize the total number of gaps and overlaps (these being given equal weight). This process may be done by hand but is time-consuming and somewhat subjective. The method given in the Appendix is a least squares method applied to the sum of the distances between vertices that originally were in contact. Minimization of this sum leads to a series of equations in the unknown translations and rotations. The equations are solved by an iterative method (see Appendix for

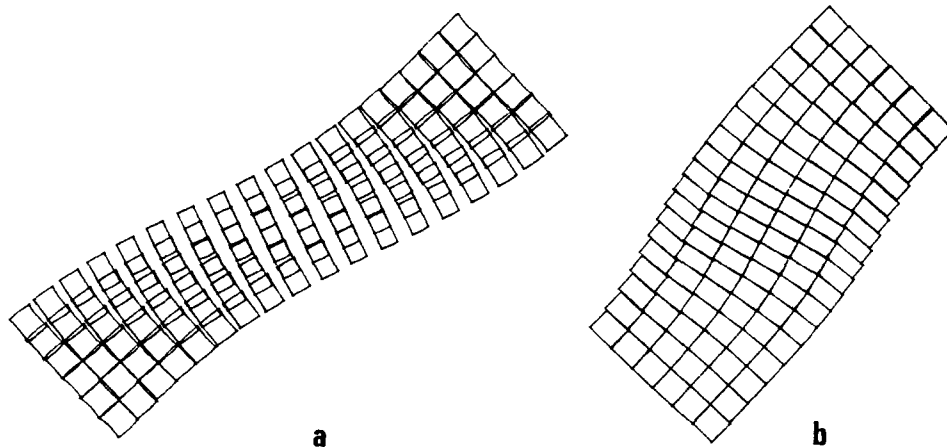


Fig. 5 Removal of shear by finite element technique. In first step (a), rectangular elements approximating those of area abcd (Fig. 3b) are unstrained without change of position or orientation, thus creating voids and overlaps. In second step (b), voids and overlaps are minimized, yielding good approximation to undeformed state (area ABCD, Fig. 3a).

details). For the example of the fold (Fig. 4b), the finite element technique gives the exact answer, because the strain trajectories in the undeformed state are in fact straight lines. For the shear zone (Fig. 5b), gaps and overlaps almost vanish completely. There is a slight imbrication of elements at the boundary of the region and this is due to the fact that neighbouring elements are missing, only a small part of the shear zone having been chosen for analysis. In the centre of the region, there is no imbrication. The results of the analysis should be compared with the exact solution (area ABCD bounded by thick outline, Fig. 3a). The approximation is quite good — sufficient perhaps for geological purposes.

5. The fifth step is the reconstruction of the finite strain trajectories in the undeformed state. These can be used to map the shape of any body from the deformed to the undeformed state, as explained in the previous section. The mapping may be performed by hand, this being perhaps as reliable as any numerical calculation.

It should be emphasized that in the tests performed using the fold and shear zone models, no errors were introduced deliberately into the strain data. A detailed evaluation of the effects of such errors is a subject for further investigation. Initial tests using deliberately incompatible elements (e.g. Fig. 6) are encouraging. If,

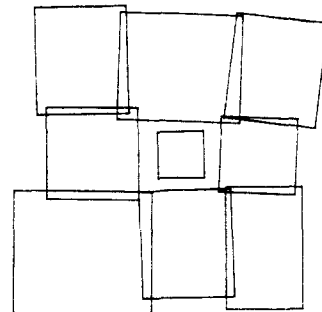


Fig. 6. Effect of local strain incompatibility. Nine finite elements are shown in positions that minimize voids and overlaps. Central element is abnormally small (incompatible) and is therefore surrounded by voids. Other elements overlap mutually to help compensate incompatibility.

for example, an element is locally too small, it will be surrounded by voids (central element, Fig. 6) whose volume can be calculated. Thus it is possible to gain a measure of errors or of local volume changes.

So far, the finite element method has been tested in two dimensions. It should be possible to extend the method to three dimensions. Another subject for investigation is the use of finite elements with curved sides. Such elements have been used successfully in finite element analysis of mechanical problems.

CONCLUSIONS

From this paper we may draw various conclusions of a theoretical and practical nature. The theoretical conclusions are as follows.

1. As a result of deformation, the strain trajectories of the undeformed state are transformed into strain trajectories of the deformed state.
2. The angle between corresponding trajectories in the deformed and undeformed states is the rigid body rotation.
3. The strain trajectories may be used as reference coordinates and for mapping from one state to the other. In terms of these coordinates, all components of shear strain vanish.
4. If the value of principal stretch is known at all points along a trajectory in the deformed state, the length of the corresponding trajectory in the undeformed state may be evaluated by simple integration.
5. If such integration is carried out simultaneously along all strain trajectories, allowance being made for rigid body rotations, the body will be restored to its original shape.
6. The presence of errors in strain data renders difficult such an integration and renders difficult also the calculation of the rigid body rotations.

Concerning the finite element method, we may draw the following conclusions.

1. Finite element methods can provide good approximations to the exact solutions for removal of deformation.
2. The method presented here includes an objective fitting of elements that is relatively rapid, flexible, and allows for the presence of errors in strain data.
3. The finite element method yields the rigid translations and rotations necessary to undeform the body in question. By fitting the elements together it also circumvents the need to integrate the deformation gradients throughout the body, and it yields directly the strain trajectories in the undeformed state.
4. The method has so far been applied in two dimensions, but should be readily applicable to three dimensional problems, which are perhaps of greater interest geologically. The two-dimensional method is nevertheless useful for undeforming folds, shear zones, or any structure formed by a general plane strain.

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APPENDIX

Fitting of elements by least squares method

The following two-dimensional method is inspired by the work of Etchecopar (1974), who used a similar approach to simulate mathematically the deformation of a polycrystalline aggregate.

The basic formulae are best derived by considering first two elements, identified by suffixes i and j (Fig. 7). The effects of more elements will be considered later. Let the coordinates of the centroids be A^i, B^i and A^j, B^j ; let the half-widths of the elements be X^i and X^j and let the half-heights be Y^i and Y^j . Initially the elements are parallel to the x, y Cartesian coordinates. The vertices are labelled 1 to 4 clockwise and the distance between vertices 2^i and 1^i is d_1 ; that between vertices 3^i and 4^i is d_2 (Fig. 7). The problem to be solved is this: if element j is rotated through an angle θ^j and the centroid is displaced to (a^j, b^j) , what is the new orientation, θ^i , of element i and the new position (a^i, b^i) of its centroid, such that the sum $D = d_1 + d_2$ is minimized?

If the coordinates of vertex 2, element i , after rotation and translation, are x_2, y_2 , then the distance D to be minimized is:

$$D = (x_2^i - x_1^j)^2 + (y_2^i - y_1^j)^2 + (x_3^i - x_4^j)^2 + (y_3^i - y_4^j)^2. \quad (1)$$

We may refer coordinates for each element to the centroid of that element by putting, for example, $x_2^i = x_2^i - a^i, y_2^i = y_2^i - b^i$. The effect of a clockwise rotation of element i on node 2 is:

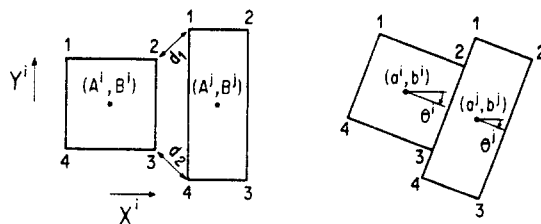


Fig. 7. Two stages in the fitting together of two elements. At left, elements i and j are parallel but separated by distances d_1 and d_2 . At right, element j has been given new position and new orientation θ^j ; element i has adopted new position and new orientation θ^i in such a way as to minimize sum $d_1 + d_2$. Elements have become parallel again and attached at boundaries.

$$\begin{pmatrix} \bar{x}_2^i \\ \bar{y}_2^i \end{pmatrix} = \begin{pmatrix} \cos \theta^i & \sin \theta^i \\ -\sin \theta^i & \cos \theta^i \end{pmatrix} \begin{pmatrix} \bar{X}^i \\ \bar{Y}^i \end{pmatrix}. \quad (2)$$

By substituting (2) and similar expressions in (1) we obtain, after much rearrangement,

$$\begin{aligned} D = & (\bar{X}^{i^2} + \bar{Y}^{i^2}) + (\bar{X}^{j^2} + \bar{Y}^{j^2}) + (a^i - a^j)^2 + (b^i - b^j)^2 \\ & + (a^i - a^j)(\bar{X}^i \cos \theta^i + \bar{X}^j \cos \theta^j) \\ & + (b^i - b^j)(\bar{X}^i \sin \theta^i - \bar{X}^j \sin \theta^j) \\ & - 2\bar{X}^i \bar{X}^j \cos(\theta^i - \theta^j) - (\bar{X}^i \bar{X}^j - \bar{Y}^i \bar{Y}^j). \end{aligned} \quad (3)$$

We now minimize D with respect to a^i , b^i and θ^i , obtaining:

$$\begin{aligned} \frac{1}{4} \frac{\partial D}{\partial a^i} &= (a^i - a^j) + \bar{X}^i \cos \theta^i + \bar{X}^j \cos \theta^j = 0 \\ \frac{1}{4} \frac{\partial D}{\partial b^i} &= (b^i - b^j) - \bar{X}^i \sin \theta^i - \bar{X}^j \sin \theta^j = 0 \\ \frac{1}{4} \frac{\partial D}{\partial \theta^i} &= -(a^i - a^j)\bar{X}^i \sin \theta^i - (b^i - b^j)\bar{X}^i \cos \theta^i \\ &+ (\bar{X}^i \bar{X}^j - \bar{Y}^i \bar{Y}^j) \cdot \sin(\theta^i - \theta^j) = 0 \end{aligned} \quad (4)$$

or:

$$\begin{aligned} a^i &= a^j + \bar{X}^i \cos \theta^i + \bar{X}^j \cos \theta^j \\ b^i &= b^j - \bar{X}^i \sin \theta^i - \bar{X}^j \sin \theta^j \\ \tan \theta^i &= \frac{(b^i - b^j)\bar{X}^i + (\bar{X}^i \bar{X}^j - \bar{Y}^i \bar{Y}^j) \sin \theta^j}{-(a^i - a^j)\bar{X}^i - (\bar{X}^i \bar{X}^j - \bar{Y}^i \bar{Y}^j) \cos \theta^j}. \end{aligned} \quad (5)$$

For this simple case of two elements, the three equations (5) may be solved simultaneously, giving $\theta^i = \theta^j$. The rotation and corresponding

translation assembles the elements as on the r. h. s. of Fig. 7. It is obvious intuitively that this pattern minimizes the distance D .

If there is more than one element adjacent to element i , then equations (5) have the same form, but each neighbouring element contributes terms on the r. h. s. in the same way as does element j . Equations (5) then give the position of element i that minimizes all gaps and overlaps with its neighbours. It can be seen that equations (5) are nonlinear in terms of θ^i , θ^j etc.

Explicit expressions for θ^i , a^i and b^i are not always easy to obtain. The equations can however be solved in an iterative way. Initial values are assumed for θ^i , a^i and b^i and new values calculated using (5). This process is repeated until no further significant change occurs in the values of these parameters. Element i is then in a best-fit position with respect to its neighbours.

For a system with many elements, each may be adjusted with respect to its neighbours, using equations similar to (5). If the adjustments are made in order, element by element, throughout the system, all voids and overlaps will be considerably reduced. Furthermore, this process may be repeated many times until the voids and overlaps are reduced no further. At this stage the solution has been obtained.

Although equations (5) are nonlinear, the iterative method of solution is closely comparable to the Gauss-Seidel method of solving linear equations. In both methods, the rate of convergence of the solution must be closely monitored, and can be hastened by suitable techniques, such as the use of an overrelaxation factor. Tests so far performed indicate that it is advisable to perform at least as many iterations as there are elements, after which further adjustments are negligible; but this general rule may not be valid in certain special situations, and care must be taken to ensure that convergence is adequate.

Computations for the model shown in Fig. 5 (108 elements) required about 4 h on a Hewlett-Packard Model 9821A Calculator. Equivalent time on a large automatic computer should be a few minutes. The array of elements was drawn by a Hewlett-Packard Model 9826A Plotter.