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1A-01 MACROMOLECULAR POSITION DETERMINATION WITH A NOISY SYNTHESIS AT LOW RESOLUTION

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If a set of diffraction data is incomplete and there are errors in structure factor phase determination, it may be difficult to find the position of macromolecule. This situation is well illustrated by Fig.1 showing a section of the function $\varrho^c(\vec{r})$ determined with the isomorphous replacement data at 4Å-resolution (all figures have been obtained when working with termitase, whose structure is being determined by E.G.Arutyunyan et al. at Institute of Crystallography of the USSR Academy of Sciences).

If $\varrho(\vec{r})$ is an exact electron density distribution, then the region $\{\vec{r}:\varrho(\vec{r})\geq\varrho^*\}$ has a quite complicate form. We consider a transform allowing a clear and simple outline of a molecule:

$\tau_R(\vec{r})$ =

= {the number of points in a sphere $|\vec{r}-\vec{u}|\leq R$ such that $\varrho(\vec{u})\geq\varrho^*$}

where R is a sufficiently large radius (of the order of molecular inertia radius). It is clear that the number of these points in the sphere is maximal when its centre is near that of the molecule. The more is the distance between the centres the less is the number.

We proposed a method of finding points at which $\tau_R(\vec{r})$ is maximal. It includes two steps. First, for each $\vec{r}$ we calculate a probability that the value at this point exceeds a critical one: $\varrho(\vec{r})\geq\varrho^*$. If we assume that the errors in determination of $\varrho^c(\vec{r})$ are normally distributed with parameters $(0,\sigma)$, then the corresponding probability will be

$$(1)\quad p_{\varrho^*}(\vec{r}) = P\{\varrho(\vec{r})\geq\varrho^*\} = (2\pi\sigma^2)^{-1/2}\int_{\varrho^*}^{\infty}\exp\{(2\sigma^2)^{-1}(\varrho-\varrho^c(\vec{r}))^2\}\,d\varrho$$

Second, for each $\vec{u}$ we calculate a mean (with respect to the introdused error probability distribution) number of points with $\varrho(\vec{r})\geq\varrho^*$ hitting the sphere of radius R with the centre at $\vec{u}$. This mean value is equal to

$$(2)\quad \hat{\tau}_R(\vec{u}) = \sum p_{\varrho^*}(\vec{r}) \qquad \text{for all } \vec{r}:\ |\vec{r}-\vec{u}|\leq R$$

Fig.2 shows the synthesis of Fig.1 modified by this procedure.

Note, that if we apply the transform (2) to the original synthesis $\varrho^{c}(\vec{r})$ without the modification (1) (Fig.3), we shall not obtain the desired result. Efficiency of this method depends on the values of ϱ^{*} and R (in our example $\varrho = 0.5 e/Å^3$, $R = 20Å$).

Fig.1

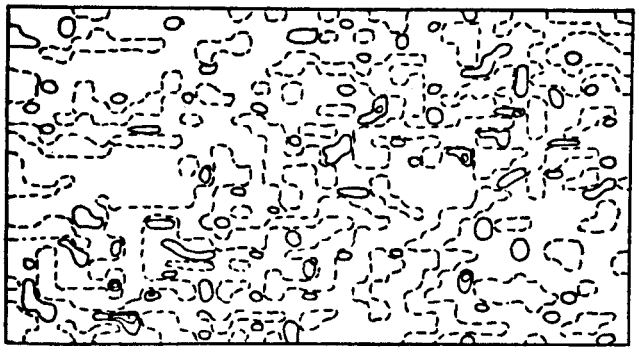

Fig.2

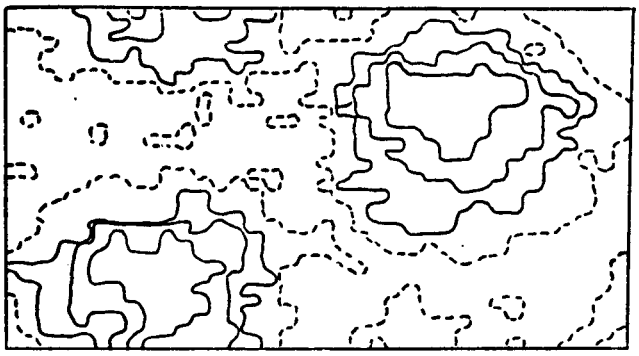

Fig.3