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The fast Fourier transform (FFT) algorithm as normally formulated allows one to compute the Fourier transform of up to N complex structure factors, $F(\mathbf{h})$, $N/2 \geq h > -N/2$, if the transform $\rho(\mathbf{r})$ is computed on an N-point grid. Most crystallographic FFT programs test the ranges of the Miller indices of the input data to ensure that the total number of grid divisions in the **x**, **y** and **z** directions of the cell is sufficiently large enough to perform the FFT. This note calls attention to a simple remedy whereby an FFT can be used to compute the transform on as coarse a grid as one desires without loss of precision.

1. Introduction

The adaptation of the FFT to compute the crystallographic Fourier transform (Cooley & Tukey, 1965; Ten Eyck 1973; Immirzi, 1973) has greatly simplified the task of producing electron density maps as well as facilitating other complex operations related to the solution and refinement of macromolecular structures. One stated limitation of using an FFT to compute a map is that sufficient storage must be allowed for the input data to perform the calculation in place. Simply stated, if the $F(\mathbf{h})$ in a one-dimensional synthesis have the vector $\mathbf{h}$ spanning the range $N/2 \geq h > -N/2$ for a maximum number N terms, the electron density $\rho(\mathbf{r})$ cannot be computed for fewer than N equispaced points, say $r = 0 \pm (N-1)/N$.

2. Discussion

This note calls attention to the simple fact that if the range of $\mathbf{h}$ exceeds the number of map grid points N, then

$$\begin{aligned}\rho(\mathbf{r}) &= \sum_{N/2\geq\mathbf{h}>-N/2} \Big\{F(\mathbf{h})\exp\big(-2\pi i\,\mathbf{h}\cdot\mathbf{r}/N\big) \\ &\quad + \sum_{n\neq 0} F(\mathbf{h}\pm nN)\exp\Big[-2\pi i(\mathbf{h}\pm nN)\cdot\mathbf{r}/N\Big]\Big\} \\ &= \sum_{N/2\geq\mathbf{h}>-N/2} \Big[F(\mathbf{h}) + \sum_{n\neq 0} F(\mathbf{h}\pm nN)\Big] \\ &\quad \times \exp\big(-2\pi i\,\mathbf{h}\cdot\mathbf{r}/N\big),\end{aligned}$$

where the quantity $F'(\mathbf{h}) = [F(\mathbf{h}) + \sum_{n\neq 0} F(\mathbf{h}\pm nN)]$ is summed to include all the observed data prior to using an FFT to compute $\rho(\mathbf{r})$ from $F'(\mathbf{h})$. This idea has been tested and proven to be accurate with no restriction as to whether the transform of $F(\mathbf{h})$ is real or complex. This appears to be the first time anyone has called attention to the possibility of computing the electron density of a structure with an FFT on an undersized grid. However, the process of computing structure factors $F(\mathbf{h})$ from a modeled density sampled on a grid-point lattice is well known to suffer from an effect called aliasing [see equation (4) of Ten Eyck (1977)]. The values of $F_{\rm calc}(\mathbf{h})$ obtained by integrating the model density on an N-point grid,

$$\begin{aligned}F_{\rm calc}(\mathbf{h}) &= \sum_{r=0,N-1} \rho_{\rm model}(\mathbf{r})\exp\big(2\pi i\,\mathbf{h}\cdot\mathbf{r}/N\big) \\ &= F(\mathbf{h}) + \sum_{n=1,\infty} F(\mathbf{h}\pm nN),\end{aligned}$$

are corrupted by an infinite series of non-vanishing higher-order terms necessary to define the model density completely. Although it is clearly not feasible to compute $\rho_{\rm model}(\mathbf{r})$ from this infinite set, it does suggest the validity of our application involving finite sums of observed data.

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References

Cooley, J. W. & Tukey, J. W. (1965). *Math. Comput.* **12**, 297–301.
Immirzi, A. (1973). *J. Appl. Cryst.* **6**, 246–249.
Ten Eyck, L. F. (1973). *Acta Cryst.* A**29**, 183–191.
Ten Eyck, L. F. (1977). *Acta Cryst.* A**33**, 486–492.