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# computer program abstracts

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## *BEAM-ish*: a graphical user interface for the physical characterization of macromolecular crystals

**Jeff Lovelace,[a] Edward H. Snell,[b] Matthew Pokross,[a] Andrew S. Arvai,[c] Chris Nielsen,[c] Nguyen-Huu Xuong,[d] Henry D. Bellamy[e] and Gloria E. O. Borgstahl[a]***

[a]The University of Toledo, Department of Chemistry, 2801 West Bancroft Street, Toledo, OH, 43606, USA, [b]NASA Laboratory for Structural Biology, Code SD48, Marshall Space Flight Center, Huntsville, AL 35812, USA, [c]Area Detector Systems Corporation, 12550 Stowe Drive, Poway, CA 92064, USA, [d]University of California, Department of Chemistry, San Diego, CA 92093, USA, and [e]Stanford Synchrotron Radiation Laboratory, PO Box 4349, MS 69, Stanford, California 94309, USA. Correspondence e-mail: gborgst@uoft02.utoledo.edu

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### 1. The crystallographic problem

Crystal mosaicity is determined from the measurement of the reflection angular width and can be used as an indicator of crystal perfection (Helliwell, 1988). A new method has been developed that combines the use of synchrotron radiation, super-fine $\varphi$ slicing and a charge-coupled device (CCD) area detector to measure simultaneously the mosaicity of hundreds of reflections (Bellamy *et al.*, 2000). Highly monochromatic unfocused synchrotron radiation of known horizontal and vertical divergence was used to minimize reflection broadening by the beam. The X-ray beam characteristics and Lorentz correction are deconvoluted from the resulting reflection widths to calculate the true crystal mosaicity (Greenhough & Helliwell, 1982).

### 2. Method of solution

*BEAM-ish* is a graphical user interface (Fig. 1) that manages the processing of multiple super-fine $\varphi$-sliced diffraction images for mosaicity calculations, seamlessly links together several programs, provides a central storage directory for files generated at all stages of the analysis, and allows the user to visualize and check the results. Data processing follows the flow diagram in Fig. 2. One or more coarse-sliced images (*e.g.* 1°) are indexed and integrated with *MOSFLM* (Leslie, 1990). The resulting `.mtz` file contains the $h, k, l, x, y, I$ and $\sigma$ of each reflection. The fine-sliced images (*e.g.* 1000, 0.001° images) are integrated by *HALFSLICE* about the detector coordinate positions for each reflection using an $I/\sigma(I)$ cutoff. For background determination, a 'seed-skewing' algorithm is used and for integration each reflection is assumed to have a radius between 2 to 6 pixels centered in a 21 × 21 pixel box. The output reflection profiles are composed of integrated intensities for each reflection for each image. The program *PEAKSTATS* then removes zingers (random radiation events), applies an optional smoothing filter, calculates reflection widths and calculates true mosaicity by deconvoluting the instrument/beam and Lorentz effects (Bellamy *et al.*, 2000). *BEAM-ish* prepares all scripts and input files and allows the user to recall an individual reflection to the screen by clicking on the reflection location on the displayed image. The data are grouped by resolution ring and/or sector for statistics calculations, and anisotropic mosaicity is calculated (Ferrer & Roth, 1998). A filtering tool is also available. Individual reflections can be fitted with several Gaussians using

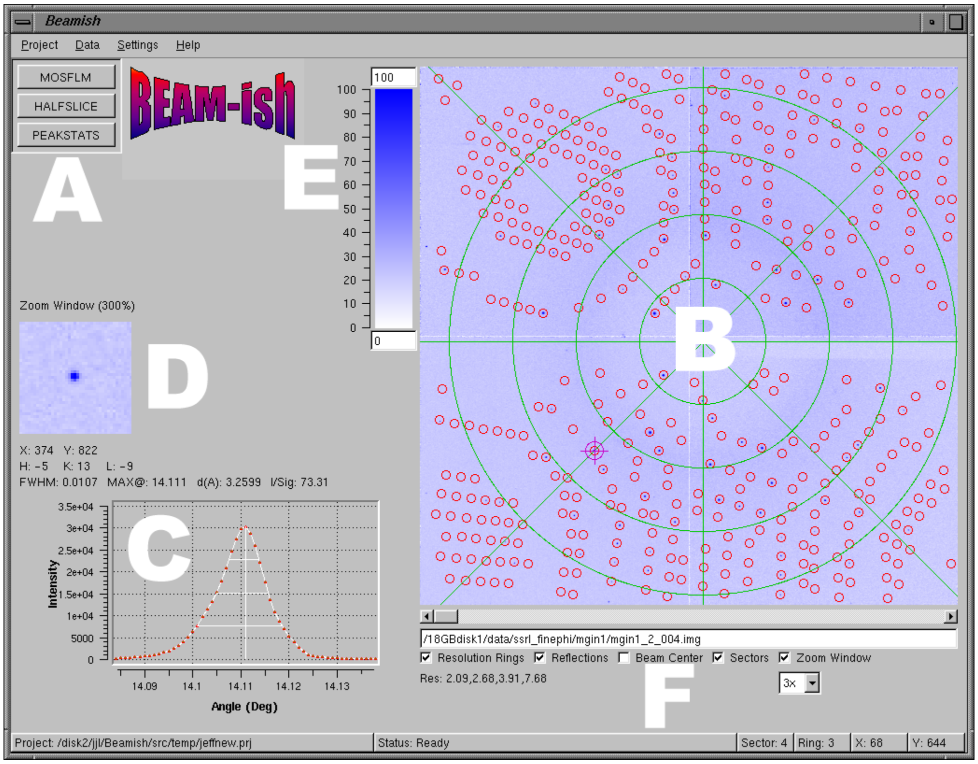


**Figure 1**
*BEAM-ish* screen elements: (*A*) data processing step buttons; (*B*) X-ray diffraction data overlaid with predictions from *MOSFLM* (small circles), resolution rings (circles) and sector definition (lines); (*C*) reflection profile display and reflection statistics; (*D*) zoom window; (*E*) user-adjustable image display scale; (*F*) detector image selection and overlay options.

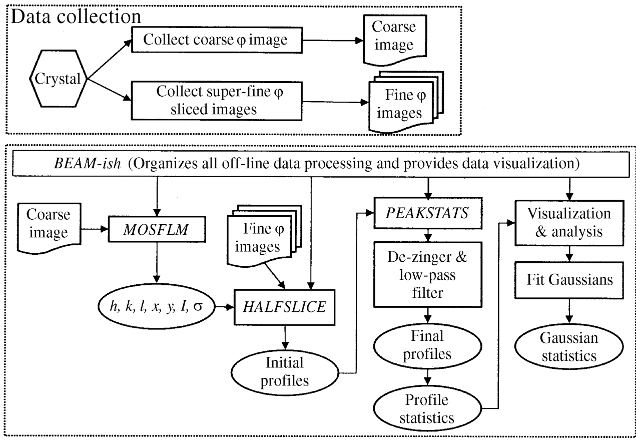


**Figure 2**
Flow diagram for mosaicity data collection and processing using *BEAM-ish*.

*MATLAB*-based (www.mathworks.com) subroutines. All output files are ASCII.

## 3. Software environment

*BEAM-ish* is designed to run under the IRIX operating system with X Windows release 11 or better. The source code for *BEAM-ish* was developed entirely in C++ and relies heavily on Troll Tech's (www.trolltech.com) *QT* library of graphical widgets. In addition, the *MATLAB* runtime library is also required to perform the Gaussian peak fitting.

## 4. Hardware environment

An O2 or better SGI workstation is needed.

## 5. Documentation and availability

Currently, *BEAM-ish*, *HALFSLICE*, *PEAKSTATS* and associated documentation are available 'as is' on a collaborative basis with the authors.

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