An extremely fast spotfinder for real-time beamline applications

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The Bragg spot analyzer described last year [*CCN* **1**, 18-23 (2010)] has been enhanced for high-throughput applications such as diffraction mapping and continual monitoring for radiation damage. The software provides raw measurements that can be harnessed by beamline developers for graphical display and instrument control. Recent work improves the program's output and performance.

Most significantly, the spotfinder package is now released under the cctbx open source license (see http://cctbx.sf.net), which now makes it independent of the packages *LABELIT* and *PHENIX*, and accessible to all beamlines worldwide. Succinct instructions for download and installation are posted at http://cci.lbl.gov/labelit, under the link for "Beamline Server". New cctbx code is tested, packaged and released on a near-daily basis; interested users are encouraged to either contact the authors with feature requests or join the cctbx open-source development group.

High-throughput performance is achieved by delegating the analysis of individual diffraction images to separate processors on a multicore CPU. The overall software architecture includes a "client" process (such as the beamline graphical user interface), which contacts the multiprocessing "server" whenever a Bragg spot analysis is required for a new image. The client, which is developed by the beamline group, can be implemented in any language (Java, TCL, Python, etc.) that supports the http: protocol needed to contact the server. In fact, it is straightforward to test the server with a standard Web browser, by requesting a URL that includes the file name of the diffraction image and any desired processing options. A simple mapping is used to convert the Unix command line for the underlying spotfinder program into a URL for the spotfinder server. Two separate implementations of the spotfinder server are now released, one using all-Python tools, and a second that uses the Apache httpd Web server for multiprocess control, within which a Python interpreter is provided by the mod-python package. The two servers give identical data analysis and similar performance, but there are some tradeoffs: the Python server is slightly easier to download and install, but the Apache/mod-python is superior in its ability to tune for peak performance. We observe the following general performance benchmarks under 64-bit Linux:

OS	Fedora 8	Fedora 13
CPU	Intel Xeon	AMD Opteron
Clock speed	2.93 GHz	2.20 GHz
# of processors	16 cores	48 cores
Overall throughput	8.9 frames/s	25 frames/s

These tests involved the processing of 720 Pilatus-6M images, with diffraction spots identified out to the corner of the detector.

Finally, many new features have been added to the spotfinder. Diffraction strength can now be summarized as a function of resolution bin, which should be of particular interest for monitoring Bragg spot quality over time from a given specimen. Additional quality measures have been added, such as background level, and signal-to-noise expressed as $I/\sigma(I)$. Numerous additional options are available for controlling the algorithm, all of which are documented on the Web page. The spotfinder work was funded under NIH/NIGMS grant numbers R01GM077071 and R01GM095887.