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19. OTHER EXPERIMENTAL TECHNIQUES



Figure 19.10.2.2

A representation of the Euler GUI tool. The three-dimensional reconstruction is shown (lower left), along with a projection and class average for a particular orientation identified in the asymmetric triangle on the right. Each cylinder in the asymmetric triangle represents a projection direction, with its height representing the number of particles found in that orientation.

permit application of any of the ~170 modular image-processing algorithms in the core library via the --process option. These include filters, masks, mathematical operations and a range of other processing algorithms. The e2help.py program provides detailed documentation for all of the modular algorithms. All EMAN2 programs are able to read automatically any of the supported file formats, and will write to any supported file format based on file extension or explicit specification of output format. For example, the command to convert a three-dimensional volume from HDF format to MRC format is simply e2proc3d.py input.hdf output.mrc.

19.10.2.3. Python wrapper

Python is an easy-to-learn scripting language in wide use in both scientific and non-scientific disciplines. It provides both an interactive prompt as well as a programming interface, and is easily extensible using higher-performance languages such as C++. *EMAN2* was designed such that all command-line programs and the entire GUI interface are written in Python. Thus, any of the distributed programs in *EMAN2* can be modified by experienced end users without a full *EMAN2* compilation environment. In addition, the program e2.py offers an *iPython*-based (http://ipython.scipy.org) interactive prompt which gives full access to all of the library functions and GUI tools of *EMAN2*. An introduction to this interface can be found at http:// blake.bcm.edu/emanwiki/Eman2ProgQuickstart.

19.10.2.4. C++

The C++ interface contains a modular system, so algorithms of various types can be trivially made available to the entire workflow system. The C++ and Python interfaces were intentionally designed to be as similar to each other as possible, so prototypes of new algorithms can be developed in Python and

Table 19.10.2.1

Listing of *EMAN2* supported file formats and whether each has read (R) and/or write (W) support

BDB refers to the *EMAN2* embedded database. DM2/3 are Gatan Digital Micrograph formats. LST files are text files from *EMAN1*.

Format	R or W support	Format	R or W support
BDB	R/W	TIFF	R/W
HDF5	R/W	PGM	R/W
MRC	R/W	PNG	R/W
IMAGIC	R/W	JPEG	W
SPIDER	R/W	LST	R/W
PIF	R/W	AMIRA	R/W
DM3	R	XPLOR	W
DM2	R	VTK	W
EM	R/W	FITS	R/W
ICOS	R/W	SAL	R

then later ported to C++. See http://blake.bcm.edu/emanwiki/ Eman2CProgQuickstart for an introduction.

19.10.2.5. Cross-platform support

All of the major computing platforms are supported, including Linux workstations and clusters, Mac OSX and Windows. Our primary development platforms are Linux and OSX. While we are committed to full support of *EMAN2* on Windows, we have encountered idiosyncratic behaviour on some specific machines running Vista which have defied explanation, but we continue to strive for full support.

19.10.2.6. Parallel processing

The three-dimensional refinement process can be extremely computationally intensive. While a refinement of a small \sim 1 MDa particle with some symmetry to 15 Å resolution may be accomplished on a single workstation in a few hours, a project like an asymmetric reconstruction to 4 Å resolution could easily require hundreds of thousands of CPU hours. Updated details of the modular parallelism strategy of *EMAN* and its GPGPU (general purpose graphics processing unit) methodology can be found in the wiki at http://blake.bcm.edu/emanwiki/EMAN2/ Parallel.

19.10.2.7. File formats and other conventions

EMAN2 supports all cryo-EM file formats for which specifications were available, in addition to its embedded database storage mechanism. While any *EMAN2* program can read and write images in any supported format, we have adopted HDF5 as an interchange format and the internal database BDB for use during workflow operations. These two permit arbitrary metadata to be associated with each image, unlike the standard cryo-EM formats. Table 19.10.2.1 contains a list of the currently supported formats.

The other primary convention of concern to single-particle reconstruction is three-dimensional orientation specification. While *EMAN2* has its own convention, it can convert to and from the most common conventions in use in the cryo-EM community, including *MRC*, *SPIDER*, *IMAGIC*, quaternions and spin axis. *EMAN*'s own convention uses *Z*-*X*-*Z*' Euler angles named az, alt and phi, respectively.