

EMAN2 Introduction

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EMAN2

- ➊ EMAN2 Wiki:
 - ➋ <http://blake.bcm.edu/emanwiki/EMAN2>
- ➋ Software Download page:
 - ➋ http://ncmi.bcm.tmc.edu/ncmi/software/software_details?selected_software=counter_222
- ➌ Discussion Mailing List/Google Group:
 - ➋ <https://groups.google.com/forum/?fromgroups#!forum/eman2>

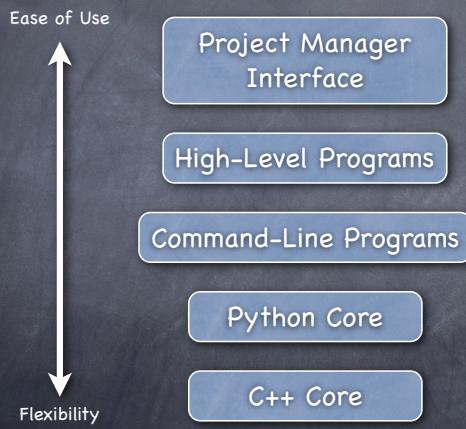
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Windows Warnings

- ➊ Windows likes to kill things
 - ➋ (killing things can corrupt databases & files)
- ➋ Windows binaries ~40% slower
- ➌ Incomplete support for parallelism on Windows
- ➍ If you want to run big reconstruction jobs, you need a Linux cluster.
- ➎ The practical reality is that structural biology software developers frequently use the command-line and rarely use Windows

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EMAN2 Architecture



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- Complete graphical workflow
- Project system which organizes data and records all reconstruction info.
- Qt/OpenGL for 2d & 3d display.
- Refinements ~5 - 20x faster than EMAN1
- Support for all documented cryoEM file formats.
- Over 200 image processing algorithms
- Use EMAN2 to launch Frealign & Relion refinements
- Tilt Validation, Random Conical Tilt, Single Particle Tomography
- Parallel processing via 3 different mechanisms
- Improved CTF correction, cont C-film, energy filter

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File Formats

BDB +

MRC	R/W	IMAGIC	R/W
SPIDER	R/W	HDF5	R/W
PIF	R/W	ICOS	R/W
VTK	R/W	PGM	R/W
Amira	R/W	Xplor	W
Gatan DM2	R	Gatan DM3	R
TIFF	R/W	Scans-a-lot	R
LST	R/W	PNG	R/W
Video-4-Linux	R	JPEG	W

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BDB Warnings

- PLEASE READ:

<http://blake.bcm.edu/emanwiki/EMAN2/DatabaseWarning>

- e2bdb.py -c
- Do NOT move files within an EMAN2DB directory around !
- If you need to remove files from an EMAN2DB directory: e2bdb.py -c
- Do NOT delete or rename directories containing EMAN2DB directories without running e2bdb.py -c first.
- If you DO get a message saying there is a database error: e2bdb.py -c
- Beware of network mounted filesystems.

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Programs

- Command-Line Programs (EMAN2)

syntax:

e2<name>.py --help
e2<name>.py <file> [--option=value] [--option] [-O]

<> - required parameter

[] - optional parameter

- e2help.py <category>

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GUI

- e2projectmanager.py - NEW workflow dialog (replaces e2workflow)
- e2display.py - General image/volume display
- e2boxer.py - Interactive particle picker
- e2helixboxer.py - Filament picker
- e2tomoboxer.py - Interactive tomogram picker
- e2ctf.py - Various CTF operations
- e2eulerxplor.py - Look at particle orientations
- e2simmxxplor.py - Evaluate how well orientations can be determined
- e2cmpxplor.py - Evaluate how different similarity metrics work

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High Level Programs

- ⦿ e2refine2d.py - reference free class-averages
- ⦿ e2initialmodel.py - Make initial models from a few class-averages
- ⦿ e2refine.py - Standard single particle analysis 3-D refinement
- ⦿ e2eotest.py - even/odd test for resolution assessment
- ⦿ e2refinevariance.py - Compute a variance map
- ⦿ e2refinemulti.py - multiple map simultaneous refinement
- ⦿ e2classifyligand.py - Split data into 2 groups based on 2 models
- ⦿ e2refinetofrealign.py - Set up for a Frealign run based on an EMAN2 refinement
- ⦿ e2runfrealign.py - Execute Frealign
- ⦿ e2refinefromfrealign.py - Process the results of a Frealign run

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Utility Programs

- ⦿ e2version.py - Display version info
- ⦿ e2speedtest.py - Test machine performance
- ⦿ e2help.py - Documentation for modular functions
- ⦿ e2bdb.py - database manipulation and querying
- ⦿ e2iminfo.py - general image information tool
- ⦿ e2proc2d.py - 2d image processing of stacks and single images
- ⦿ e2proc3d.py - 3d image processing of 3-D stacks and single volumes
- ⦿ e2parallel.py - Used for some parallelism operations
- ⦿ e2.py - Python command-line for EMAN2

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Extensible Core

Type	Description	#
Processor	Generic image processing algorithms, filters, masks, thresholds, etc.	175
Aligner	Algorithms used to align 2 images or volumes to each other	22
Projector	Routines to generate 2-D projections of 3-D objects	6
Reconstructor	Routines to reconstruct 3-D objects from 2-D projections	11
Cmp	Similarity metrics used to compare two images or volumes	10
Averager	Average together stacks of images in various ways	7
Analyzer	Perform various operations on sets of images, such as classification or PCA	6
Orientgen	Routines describing how projections cover the asymmetric triangle	6

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Processors

(categories & examples)

- filter
 - filter.lowpass.gauss
 - filter.homomorphic.tophat
- mask
 - mask.sharp
 - mask.gaussian
- math
 - math.sqrt
 - math.laplacian
- misc
 - misc.localnorm
- normalize
 - normalize
 - normalize.edgemean
- testimage
 - testimage.scurve
- threshold
 - threshold.binary
 - threshold.clampminmax
- xform
 - xform
 - xform.centerofmass
 - xform.fourierorigin.tocenter

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Similarity Metrics

(cmp)

With Default options, SMALLER → more similar

- dot - dot product (negative by default)
- frc - Fourier ring correlation (weighted)
- optvariance - 'optimized variance' (EMAN1)
- phase - mean phase error
- quadmindot - Worst of quadrant dot products
- sqeuclidean - sum $(a-b)^2/n$

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