
Desirable Software Components for Structural Biology



Pam Thuman-Commike
pam@qedlabs.com

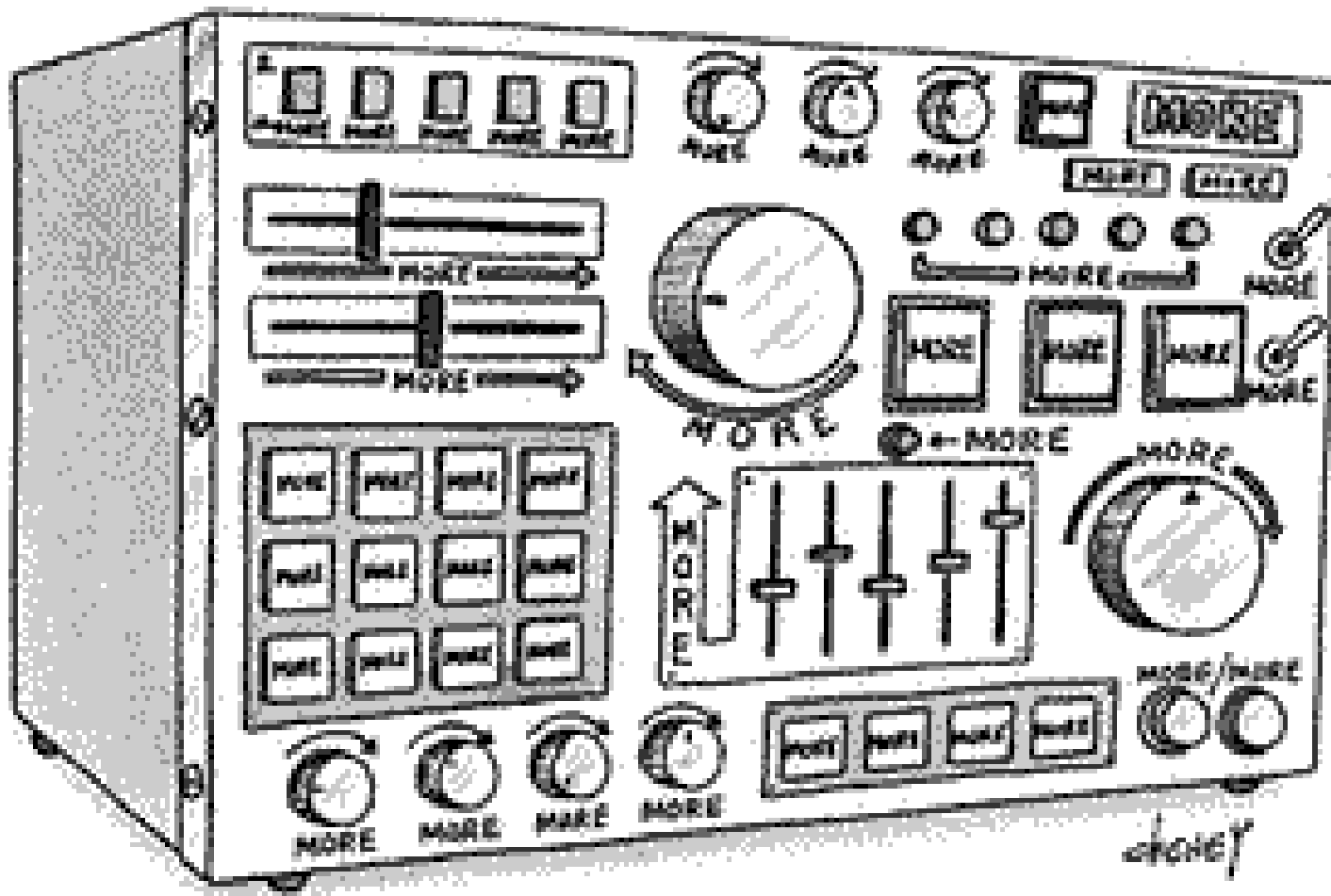
EM Software Capabilities

- Extensive and growing capabilities in a wide range of software
 - Particle selection
 - Single particle structure determination
 - Structure animations
 - Structure modeling
 - Structure visualization

Science is always demanding more

- More accuracy
- More speed
- More features
- More visualization

More, more, more....



More Software

What about

- **more intuitive?**
- **more assistance?**
- **more flexible?**
- **more configurable?**

More usable software!

What makes software difficult to use?

- **A painful, frustrating or hair pulling experience!**

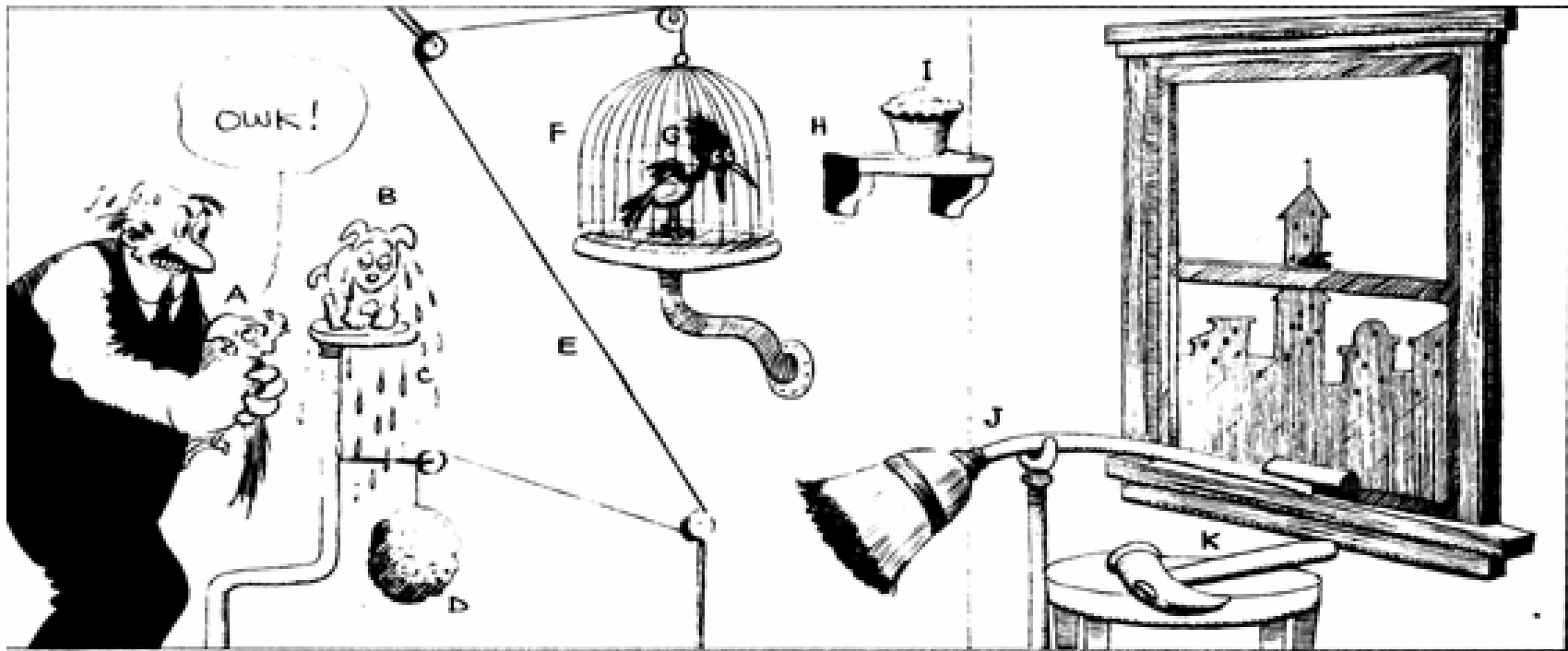
Using software shouldn't be Torture!



"I need someone well versed in the art of torture—do you know PowerPoint?"

What makes software difficult to use?

- A painful, frustrating or hair pulling experience.
- **Overly complex - requiring repeated confusing actions!**



After trying to open window for ½ hour, you relieve your anger by choking Parrot (A). Dog (B) hears Parrot's groans and weeps out of sympathy – tears (C) soak sponge (D) causing its weight to pull string (E) which lifts top off cage (F) releasing wood pecker (G) which chews away shelf (H) causing heavy biscuit (I) to fall on broom-handle (J) thereby acting as a lever in raising window. **After repeating this 6 times without success, take hammer (K) and break glass in window allowing fresh air to enter room!**

What makes software difficult to use?

- A painful, frustrating or hair pulling experience.
- Overly complex - requiring repeated confusing actions!
- **Hidden Features.**

What are the software features?

File	Menu 2	Menu 3	Menu 4	Menu 5	Menu 6	Menu 7	Menu 8

What makes software difficult to use?

- A painful, frustrating or hair pulling experience.
- Overly complex - requiring repeated confusing actions!
- Hidden Features.
- Lack of interactive assistance to aid user in usage.

Lack of guidance for user

File	Menu 2	Menu 3	Menu 4	Menu 5	Menu 6	Menu 7	Menu 8

What makes software difficult to use?

- A painful, frustrating or hair pulling experience.
- Overly complex - requiring repeated confusing actions!
- Hidden Features.
- Lack of interactive assistance to aid user in usage.
- **Requires expert assistance in order to use.**

Expert is not built-in

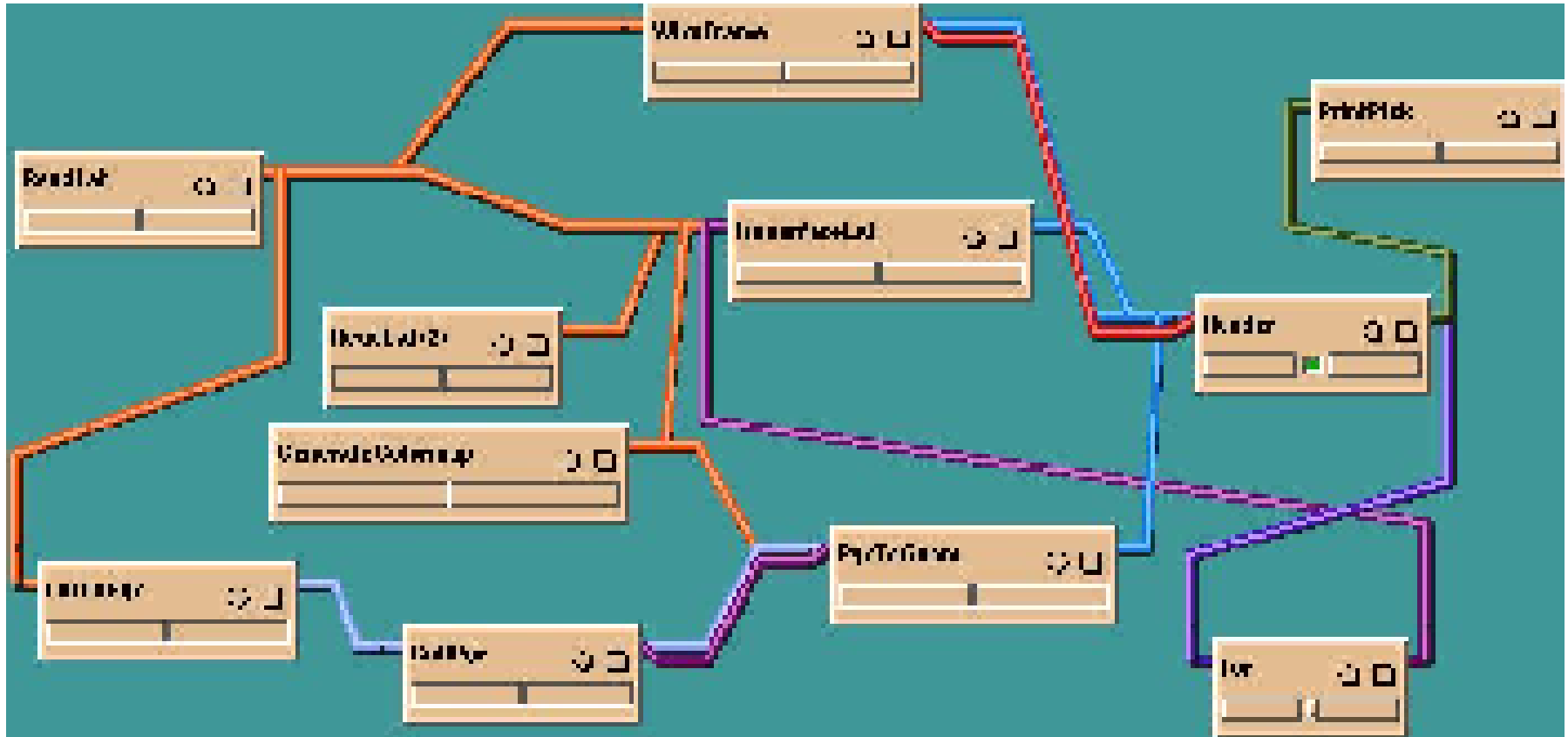


Software should just be usable by all users without assistance!

What makes software difficult to use?

- A painful, frustrating or hair pulling experience.
- Overly complex - requiring repeated confusing actions!
- Hidden Features.
- Lack of interactive assistance to aid user in usage.
- Requires expert assistance in order to use.
- **Capability without access.**

Toolkits Only Benefit Experts



Software should help you use it....



What is easy to use software?

- Not a painful, frustrating or hair pulling experience!
- It is not overly complex.
- Features are obvious and accessible.
- It provides interactive assistance on usage.
- Doesn't require expert assistance.
- It is flexible and configurable.
- Enjoyable and productive to use

Allow non-experts to accurately perform data processing.

One approach to usable software

- **Guidance:** Aid user in determining what, when, why and how to perform actions and process data.

**To allow complex data processing
to be performed by non-
specialists.**

Details on performing computations

- Guide users on necessary steps
- Explain when to perform steps, how to perform them and why to perform them
- Provide alternative pathways for achieving results
- Provide mechanism for user to determine appropriate pathway based on their underlying data

Details on performing computations (cont.)

- Make parameters accessible
- Provide descriptions of what parameters mean, how to choose them, and when to change them
- Provide mechanism for user to determine appropriate values based on their underlying data

Next Guidance: What to do and When to do it

- Indicates current and next step providing user what to do and when to do it.
- Dynamically updates as user performs data processing
- Details
 - How to do the steps
 - Why to do the steps
 - When to do the step

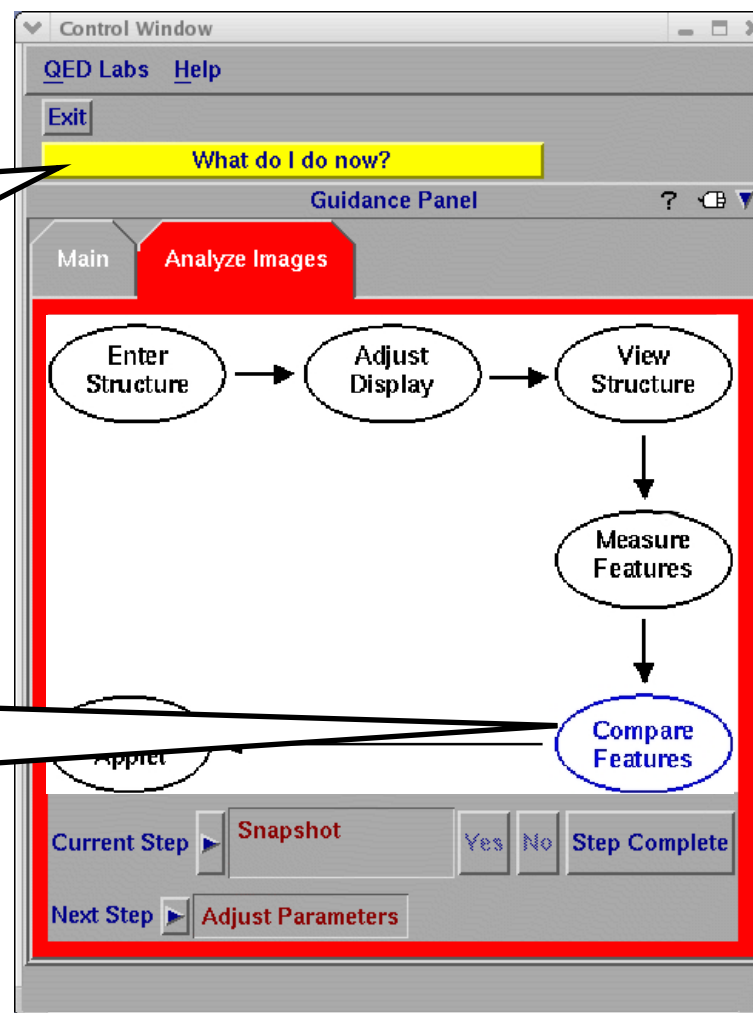
Next Guidance: Data Processing Cycle

PANIC BUTTON:

Obtain immediate help on current task

CURRENT STEP:

Bubble indicates current step



Next Guidance:

“Why and how to do this?”

- Details on why steps are necessary with references to publications providing further details.

Next Guidance for Feature Extraction

What does this step do?

The step is to perform feature extraction on the particles with the structural study.

Feature extraction is performed to identify commonality within the image set and reduce the complexity of the images. The commonality is identified by performing multivariate statistical analysis that describes the images using a set of Eigenvectors that denote the most common features of the images. The Eigenvectors themselves result from an analysis of the covariance matrixes computed between every pair of image pixels in the entire dataset. The complexity reduction results by limiting the common image features to the most important Eigenvectors and representing each image as a product of the Eigenvectors and the original image pixels. Overall feature extraction facilitates classification by providing the features on which to classify and by reducing the number of variables per image (i.e. rather than $N \times N$ pixels the image is represented by NumEigen pixels).

Why do I need to do this step?

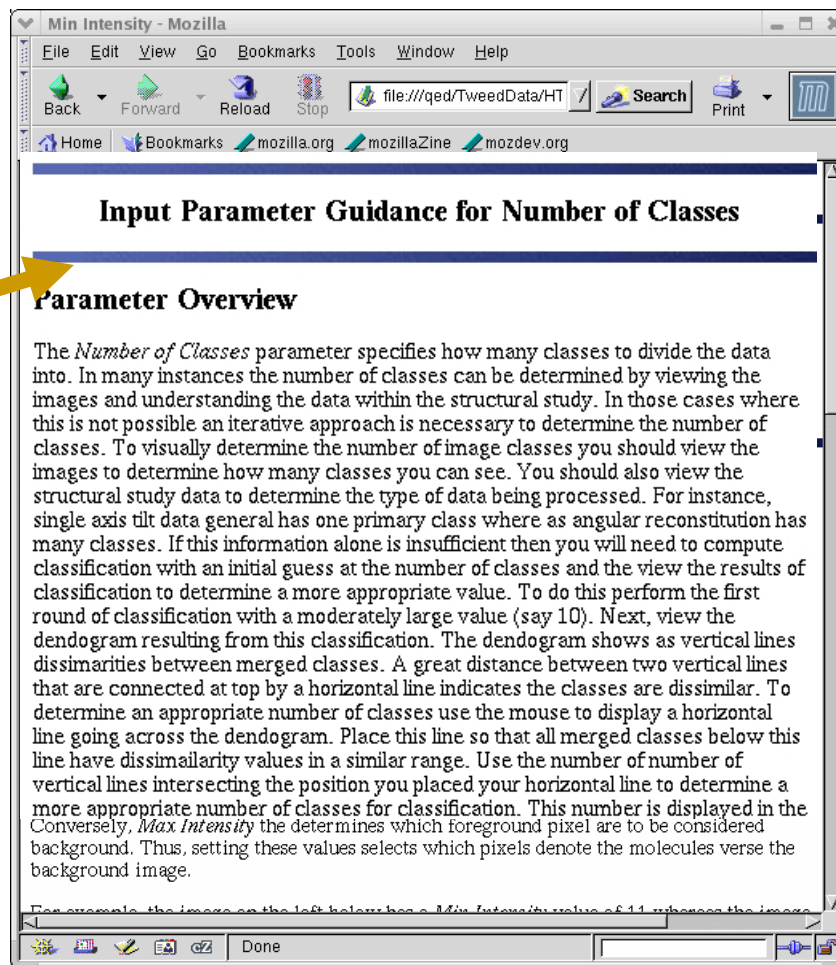
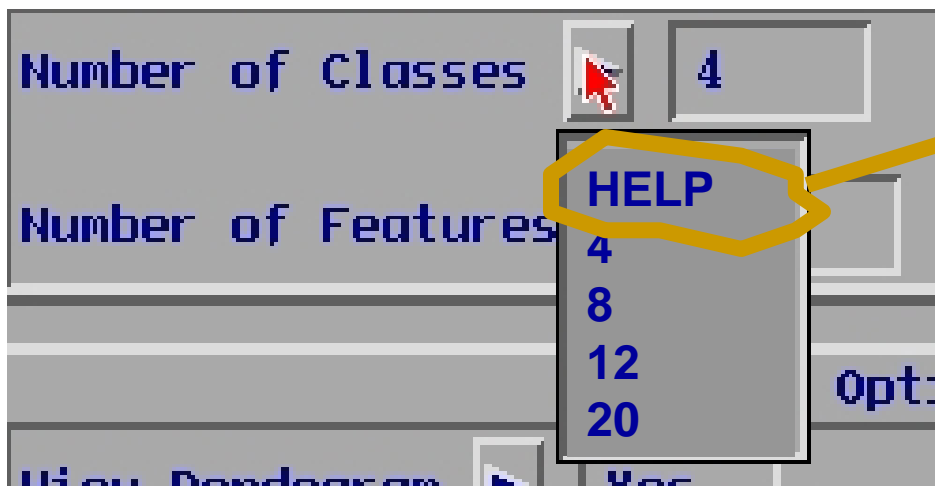
Feature extraction is a requirement of image classification. Electron microscopy images are noisy with many features. Classification of the original images is inaccurate and slow. Feature extraction is a preprocessing step that reduces the size of the images and extracts the most common features of the images making classification more accurate and quick. Once you have viewed the images the next step is to perform feature extraction in preparation of classification.

How do I do this step?

Input Parameter Guidance

- Compute suggested parameter values based on data and current results
- Provide summary of how to choose parameter values and understand effects of those changes
- Values are computed dynamically - not hard coded

Input Parameter Guidance



Summary

- **Goal: Easy to use software by all users not just experts in the data processing.**
- Users should **demand**
 - Software that helps you use it
 - Software that is enjoyable to use
 - Software that is flexible/configurable

