



Introduction

MacroScopeJ is a desktop application used for examining crystallization experiment images and data. It is intended as an upgrade/replacement for HWI's original MacroScope program. MacroScopeJ is an ongoing project which will be improved and extended in future releases.

About this release

While MacroScopeJ shares much functionality with our earlier program, it is intended to far surpass MacroScope's capabilities. In order to make this possible, it was necessary to create a new interface, change features, and add new features.

The current release aims to supersede MacroScope by providing all existing functionality, while introducing the new interface of MacroScopeJ and many of the new tools that have been developed. Some major changes include:

- Cross-platform Java technology
- Multiple-document interface
- Improved navigation controls
- Image thumbnail resizing
- Color-coded scoring
- New tools, such as magnifying glass, crystal measure, and slideshow

Some features are intended to be upgraded or enhanced in future releases. This release operates only in a "Legacy" mode which mimics existing MacroScope features, such as loading/saving MSO files, extracting cocktail data from composite lists, and exporting HTML pages. Future versions will also include a limited-feature Legacy mode; but emphasis will be on developing a new, more comprehensive data-centric base.

For existing MacroScope users

It is important to keep in mind that MacroScopeJ is not merely the next release of MacroScope; it is a new and different program. It contains a completely new code base, written in a different language, and was designed with a much broader scope of goals in mind. It is therefore, of necessity, a much more complex application than MacroScope. To become acquainted with the new design and features, take the time to read the section entitled "Concept overview".

That being said, much of the program will appear familiar to the veteran MacroScope user. There are still two essential experiment views: a page of well thumbnails, and a full-size image review window. For those who score their images, the scores may be toggled using the same 7 numpad keys. There are again several export options, including the traditional MSO (**MacroScope Output**) file and HTML web page. To help you get started, there are tutorials at the end of this document explaining how to perform some basic tasks that you have probably done before using MacroScope. Other features and tools can be explored at your leisure.

There are some particulars that should be noted:

- When opening an MSO file, MacroScopeJ first looks for the required RAR file in the same directory. If it cannot be found there, the program will ask you to browse for it manually.
- Image thumbs are arranged, by default, in order of sequential well position #, not cocktail #. (This can be changed inside the “Visual Elements” tab of the arrangement’s “Tools” panel.)
- Image thumbs also, by default, display the well position #. (This text can be hidden or changed to display the cocktail # using the “Visual Elements” tab.)
- “Selecting” an image in MacroScopeJ is essentially the same as “marking” it in MacroScope, though it is more flexible because of the options provided throughout the program.
- There are two web page export formats. “HTML Selection List” is the one most similar to MacroScope’s “Save as web page” feature.

System requirements

- Java-capable OS (officially tested on the following systems, though others may also work:)
 - Windows XP
 - Windows Vista
 - Windows 7
 - Mac OS X 10.5 “Leopard”
 - Mac OS X 10.6 “Snow Leopard”
 - Ubuntu 9.04 “Jaunty Jackalope”
 - Ubuntu 10.4 “Lucid Lynx”
- Java Runtime Environment (JRE) 1.6 or later
- 256 MB of available RAM*
- 1.60 GHz. processor or faster recommended†

*256 MB is the default/recommended maximum amount of RAM for the JVM (Java Virtual Machine) in which MacroScopeJ runs. The default JVM heap settings (min: 128MB – max: 256MB) should be sufficient for most users. If you are using a powerful machine with lots of RAM, you can change these settings by running MacroScopeJ from a console (terminal or command prompt).

The following example will launch MacroScopeJ with an initial heap size of 128MB and a maximum of 1024MB:

```
> java -jar -Xms128m -Xmx1024m MacroScopeJ.jar
```

†Intel Atom @1.60 GHz is the minimum processor that MacroScopeJ has been tested on. You can probably use a slower processor if you want; of course, MacroScopeJ will be... well... slower.

Support

Support is provided by the developer. He can be reached at (716)-898-8676 or rnagel@hwi.buffalo.edu. The best way you can help us to make MacroScopeJ better for you is providing detailed feedback. If you receive error messages, or a feature does not behave as expected, please:

1. send a description of the error and what you were doing when it occurred
2. provide information about your operating system, Java version, and MacroScopeJ version
3. attach screenshot(s) of the problem
4. be prepared to assist in troubleshooting the problem

Concept overview

(This section lists some of the important concepts in MacroScopeJ. It is advised to read this section before following the tutorials at the end of this document.)

Projects & Legacy Mode

MacroScopeJ is intended to work with *Projects*, collections of related files that are stored, opened, and saved as a complete unit. Projects have been disabled for this release; instead, there is a type of pseudo-project called “Legacy”. Any open arrangements will be stored in the “Legacy” folder in the “Projects” tab.

Resources

Resources are external files which are used by MacroScopeJ, but not loaded into memory; instead, their locations are manifested so that they can be accessed by the program when required. In this release, the only type of resource is RAR archives. When a RAR file is loaded, its content is extracted to a temporary location, and it is displayed as an icon in the “Resources” panel at the left side of the main window. Henceforth, any arrangement or feature (e.g. history) that requires the contents of the RAR file will be able to access it.

Right-clicking a resource icon in the “Resources” panel will give the user several options: notably, “Unload” and “Delete”. The *unload* option will clean up any temporary files extracted from the resource, and remove the pointer to the resource file. To use the resource again, it must be reloaded. If an existing arrangement cannot find a RAR file because it has been unloaded, it will display “Image not found” instead of the image. (Note that all resources are automatically unloaded when MacroScopeJ is exited.) The other option, *delete*, will literally delete the resource file from disk. It is a convenient shortcut for removing a local copy of a file that is no longer needed. Use caution, and **NEVER SELECT THIS IF YOUR RESOURCE IS A UNIQUE, ORIGINAL FILE ON YOUR COMPANY’S ARCHIVE SERVER!!!**

Arrangements

Arrangements are the features which contain and display the images you work with. In this release, all arrangements contain, by default, every image from a particular RAR file. Thumbnails are displayed one page at a time; there are 16 pages, each with 96 images, for a 1536-image RAR file. The currently

displayed page can be changed with the controls at the top of the arrangement frame. Left-clicking an image will bring it up in the full-image window. Right-clicking an image will select it within the arrangement.

Tools

When an arrangement's frame is active (focused), the "Tools" panel on the right side of the main window will display tools for manipulating the arrangement. Click the appropriate tab to view/change options for a particular tool.

Currently available tools include:

- cell (image) sizing
- mouse functions
- selection options
- visual elements
- slideshow
- transform/export

Selection

Images can be selected in the arrangement by right-clicking them. To select a contiguous group of images, right-click an unselected image and drag over the other images. Deselecting images is performed the same way, except that you right-click on an already selected image. Options for selecting can be changed in the "Selection" tab in the "Tools" panel. The selection can also be hidden by unchecking "Show selection" in the "Visual Elements" tab. An image may also be selected by pressing the spacebar while in the full-image window.

Selection has a number of uses. It can be used to mark images to be reviewed later, or to specify which wells should be saved in an MSO file. It can also be used to limit the images used in an operation, such as viewing a slideshow.

MDI Interface

MacroscopeJ has been designed with a multiple-document interface, meaning that multiple documents can be open at once. Thus you can have several arrangements open within MacroscopeJ, each in a separate internal window, as opposed to having several instances of the application open simultaneously. All open documents are shown as icons in the "Projects" panel. (In this release, the only type of document is *arrangement*.) Right-clicking a document icon will give the user several options: show, close, rename, delete. *Show* will ensure that the document's window is visible in the main desk area. *Close* will close the document's window (the document will still be in memory). *Rename* will change the name of the document. *Delete* will remove the document from memory. There are several window operations available for working with open documents; these are available in the "Window → Arrange" menu, and on the icon bar for convenience.

(Note that all documents are automatically deleted when MacroScopeJ is exited. Projects are disabled in this release, which means that documents cannot be saved as such. To save your work, you should choose one or more export formats from the “Transform” tab in the “Tools” panel: see tutorial #4.)

Full-Image Window

Left-clicking a thumbnail in an arrangement will show the full-sized image in another window. This window is most useful for checking images one at a time for crystallization outcomes. Depending on how the software is used, this may be done by selecting the image or by categorizing it using one or more “scores”. This window, like the main window, contains a toolbox on the right side; selecting a tool’s tab will enable that tool (which sometimes uses the mouse) and show options for it. For more information on using this window, see tutorial #2. For information on using the well history tool, see tutorial #3.

Memory

As any Java program, MacroScopeJ runs within its own Java Virtual Machine (JVM). The JVM is set up to work with a finite allocation of your system’s memory (RAM). The default for MacroScopeJ is 128MB (minimum/initial allocation) to 256MB (maximum allocation). The more arrangements (or memory-intensive operations) you have open at one time, the more memory will be used. From time to time, Java will automatically “collect garbage”, i.e. free up memory which is no longer being used.

In the main icon bar, there is a meter icon that displays a percentage: this is the amount of currently used memory in relation to the maximum amount available to the JVM. When this percentage approaches 100%, the application is in danger of crashing. It is the user’s responsibility to monitor this number and work with only a manageable number of documents at any time. If you find it necessary, you may increase the amount of memory allocated for the JVM (see the “System Requirements” section of this documentation for more information).

Clicking the memory icon (or pressing Ctrl+M) will display a memory monitor dialog, which shows a more detailed analysis of JVM memory usage. You can also click a button to “force garbage collection”.

Launching the application

For Windows users: Run “MacroScopeJ.exe” (Windows executable)

For Mac users: Run “MacroScopeJ.app” (Mac application)

For Linux users: Run “MacroScopeJ” (bash script)

(For some support calls, the user may be instructed to run “MacJLog.bat”, or to start MacroScopeJ from a command prompt or terminal. This produces log and error information that can be useful to the developer to diagnose issues.)

Basic Operation

(This section will guide a new user through using MacroScopeJ to review and select images of interest, and then to export the selection as an MSO file. Follow these steps when requesting additional HTS Lab services, such as UV imaging.)

<p>1. Start MacroScopeJ. (See above section on “Launching the application”.)</p>	<p>2. Select “(Legacy) Open MSO/RAR” from the “File” menu.</p>
<p>3. Browse for the RAR file. The default filter shows both RAR and MSO files. To view only RAR files, select the appropriate filter.</p>	<p>4. The RAR file will be extracted. Notice that it is now listed in the “Resources” panel on the left. Also, a new <i>Arrangement</i> has been automatically created to show you the RAR’s images.</p>
<p>5. Left-click the first image in the arrangement; this will create a popup window showing the image at full size.</p>	<p>6. If the image looks interesting, press spacebar to select it. This tells the program that the image should be exported when the MSO file is created. Press → or [Enter] to move on to the next image.</p>
<p>7. When you are finished reviewing images, close this window. Go to the last tab of the main Toolbox and click the button to export as “MSO File”.</p>	<p>8. Browse to the location where you want to export the new MSO file and click “Save”. On the following dialog, leave the default options checked and click “OK”.</p>

Other Tutorials

(These tutorials do not attempt to cover the full range of current MacroScopeJ features. If you notice that a feature or option is not mentioned in this documentation, experiment with it.)

#1: Open a single RAR file to view its images

1. Run MacroScopeJ.
2. Select “(Legacy) Open MSO/RAR” from the “File” menu.
3. Browse for the RAR file. The default filter shows both RAR and MSO files. To view only RAR files, select the appropriate filter.
4. The RAR file will be extracted. Notice that it is now listed in the “Resources” panel on the left. Also, a new *Arrangement* has been automatically created to show you the RAR’s images.
5. Right-clicking on an image will *select* it within the arrangement. To select more than one image, right-click and drag across the images. To deselect, right-click on an already selected image.
6. You can use the tools in the “Tools” panel to interact with your new arrangement of images. Change tools by selecting a different tab, and try them out!
7. By default, the arrangement puts a RAR’s images in 16 pages, each with 96 images. You can use the drop-down box or arrow buttons at the top of the arrangement window to view other pages.

#2: Viewing single images full-size in a popup window

1. Left-click on any image in the arrangement; this will create a popup window showing the image at full size.
2. You can navigate to the previous or next image in the arrangement by clicking the arrow buttons in the “Navigator” frame, or using the left/right arrow keys. Press “Home” to jump to the first image in the arrangement, or “End” to skip to the last image.
3. To navigate through only selected images, click the red arrow buttons or press [Ctrl] + [left, right, home, end].
4. To optimize the display for small screens (such as netbooks), this window may be automatically resized. If the well is not properly centered in the “Image” frame, you can use the scroll bars to position it. The position will remain when you change to other images.
5. To view cocktail data (composite list entry) for the image, check “Show Composite list data” from the “File” menu. A new always-on-top window will appear; you can drag this and resize it as desired. The data will be updated when you change to a different image.
6. To toggle whether the image is selected in the current arrangement, press the space bar. When an image is selected, you will see a red flag in the top-right corner of the image.
7. To score the image, select the “Scoring” tool from the “Toolbox” frame and check the box for the score you want. You can also press the corresponding number key on your keyboard to toggle the score. Multiple scores are allowed; note, however, that “clear” is exclusive.
8. You may exit this window by closing it with the mouse or by pressing the Escape key.

#3: Viewing well history

1. First open an MSO or RAR file to produce an arrangement of images (see tutorial #1).
2. Select “Load Resource(s) → Load RAR File(s)” from the “File” menu.
3. Browse to locate RARs for the other reads that you want to include in the history view.
4. Each RAR file is extracted and added to the “Resources” panel on the left.
5. Left-click an image to open the full-size window.
6. Select the “History” tab from the “Tools” panel. You will see a thumbnail of the well for each read, along with a timestamp.
7. Mouse over the history thumbnails to view the full-size image of the read.

#4: Exporting an arrangement

1. In the main window, activate the arrangement you want to export. The “Tools” panel on the right will display arrangement tools.
2. Select the last tab, “Transform”.
3. There are three options available:
 - a. Export as MSO File
An MSO file is a plain text file which saves the composite list entries for selected images/wells. Any scores will also be saved. This is a backwards-compatible file that can be opened in MacroScope, AutoSherlock, etc.
 - b. Export as HTML Arrangement
This option saves a folder containing an HTML version of the arrangement. You can either save the current page of images, or the entire arrangement with an index + 16 pages. When opened in a browser, you will see the images arranged as in MacroScopeJ; left-clicking a thumb will show you the full-sized image (with composite list info) in another window/tab. You may also choose to “create true thumbnail images”, which will make the loading time for each page faster when viewing online (at the expense of storage space).
 - c. Export as HTML Selection List
This option saves a folder containing an HTML list of the currently selected images. When viewed in a browser, you will see a table containing image thumbs, composite list data, and any scores. Left-clicking a thumb will show you the full-sized image (with composite list info) in another window/tab. You may also choose to “create true thumbnail images”, which will make the loading time for each page faster when viewing online (at the expense of storage space).
4. If you plan to import the scores into MacroScopeJ (or another program) at a later time, export an MSO file. If you want to show an entire page, or all pages, in a browser (rather than in MacroScopeJ), export an HTML arrangement. If you want to view certain wells in a browser, possibly online, export an HTML selection list.

Operating system notes

MacroScopeJ was developed on Microsoft Windows Vista and Windows 7, 64-bit editions. As a PC running Windows is today's *de facto* standard, this documentation has been written with the Windows user in mind. If you are using a different operating system, the following notes may be useful to you.

Mac OS X:

- Every version of Mac OS X comes with Java pre-installed. Earlier versions of Mac OS X come with Java 5 (J2SE 5.0). You can check your current Java version by typing "java -version" from Terminal. MacroScopeJ requires Java 1.6 or later to run. If your current version is not 1.6, open your "Java Preferences" and set 1.6 as your default (if present). For more information about Java on Mac OS X, see <http://developer.apple.com/java/faq/>.
- This document assumes that you have a mouse with at least 2 buttons. If you are using an Apple mouse with only one button, you may be able to simulate a "right-click" by using "Ctrl+click".

Linux:

- MacroScopeJ has been tested on 2 versions of Ubuntu, which is by far today's most popular Linux distribution. Hopefully it will also run on other distributions without a problem; but no other distribution has been tested yet.
- Running MacroScopeJ on Linux may require you to install UnRAR separately. If your distribution uses a package manager (Debian, etc.), it is advised that you use it to install UnRAR. Otherwise, you may be able to obtain it from the RARLAB website: http://rarlab.com/rar_add.htm

Other:

- Other operating systems may have Java installed and be able to run Java programs; however, at this time, they are not supported by MacroScopeJ. This is because MacroScopeJ requires the UnRAR program, which is only included now (along with the respective free license files) for certain operating systems. If we receive enough requests for another OS, we will consider extending support for it in a future release.