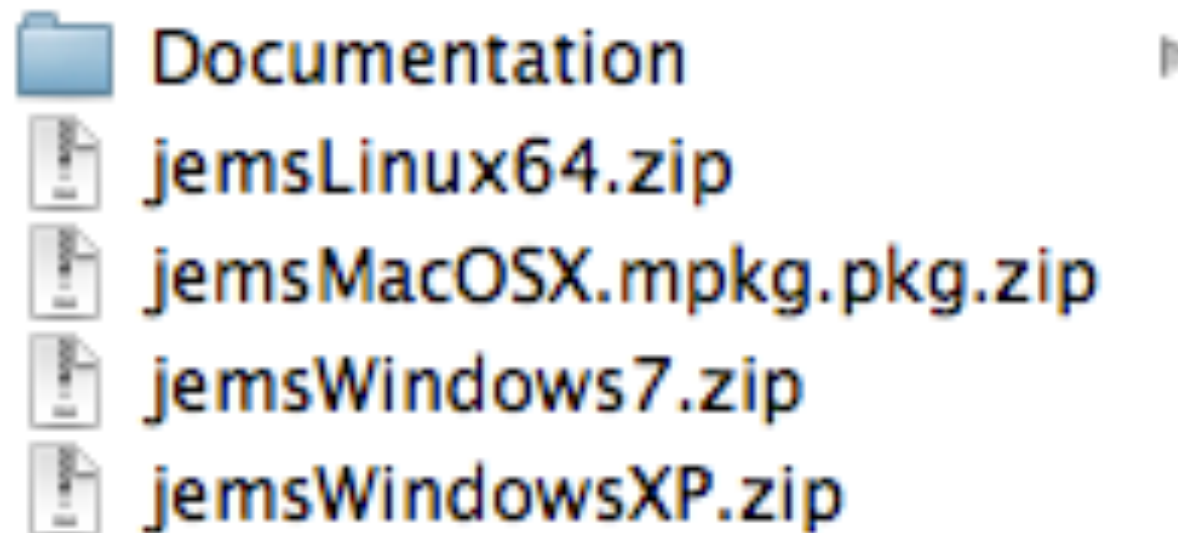


# TD Simulation

Ecole Nord Africaine et workshop en Microscopie Electronique

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- ▶ Copy the .zip file compatible with your PC operating system.
- ▶ Do not open it, but use Extract All in order to unzip the file.

# Extracting jems

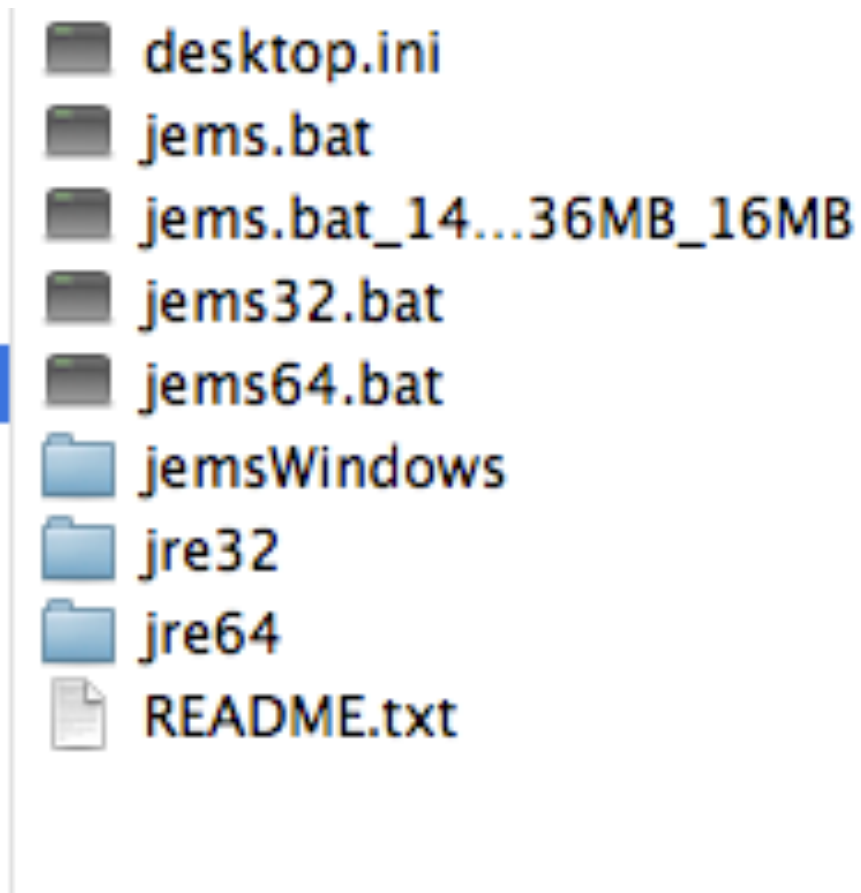


Figure: Windows 7 or 8 version: jems started either using jems32.bat or jems64.bat depending on Windows being 32 or 64 bits.

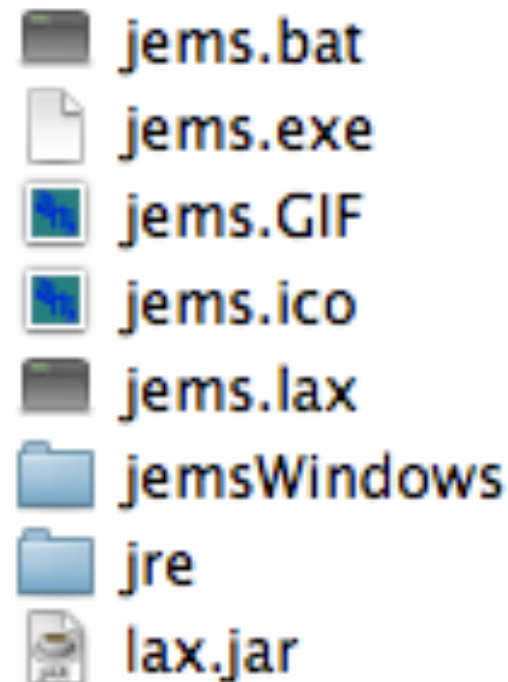


Figure: Windows XP (only 32 bits).

For Windows 7 after having determine the version 32 (or 64) copy jems32.bat (or jems64.bat) to jems.bat. jems modifies jems.bat.

# Starting jems

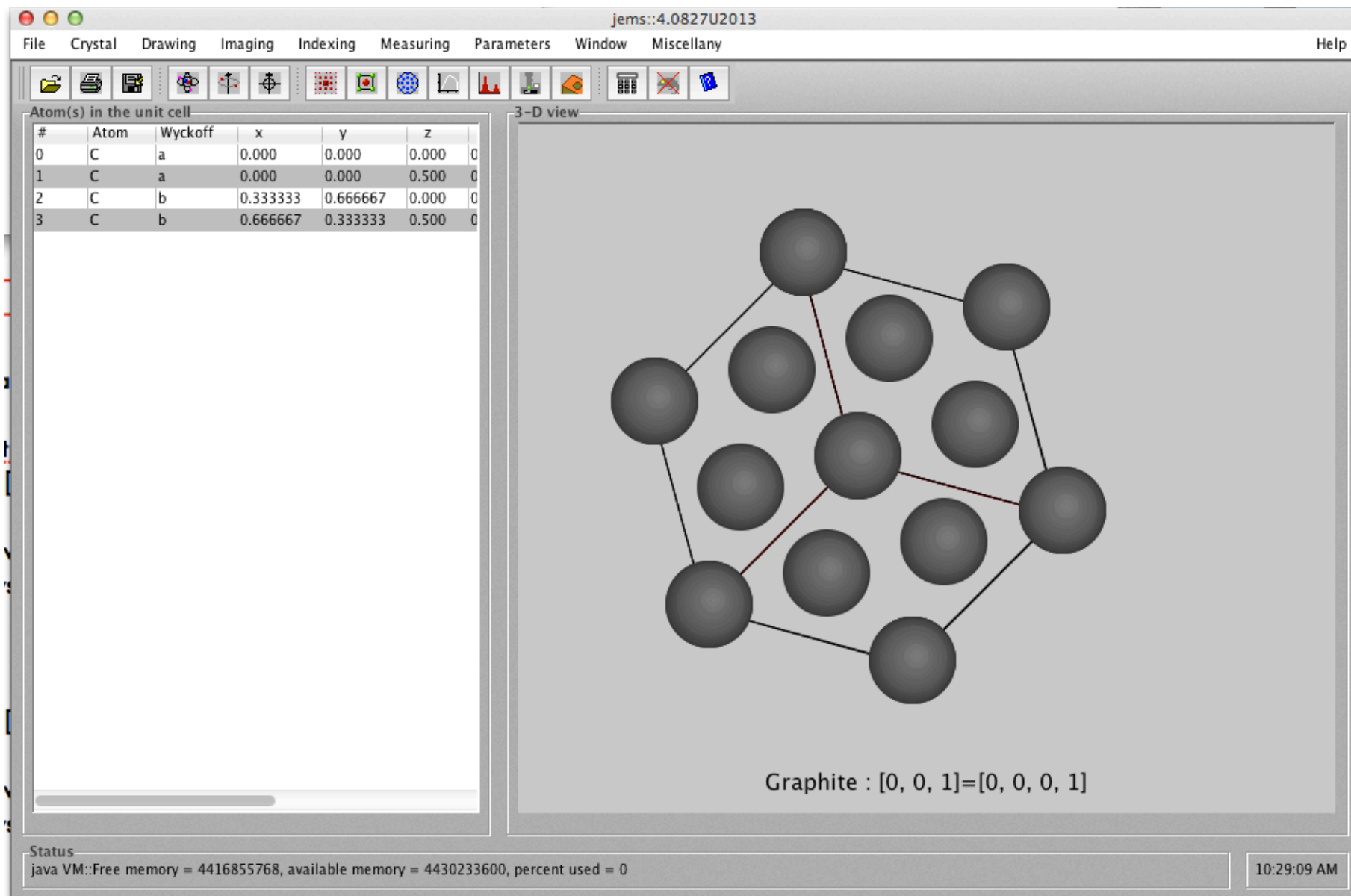


Figure: Starting jems you will get error messages: do not exit jems but open the [License dialogue](#) (License menu item of Help menu).

# License dialogue

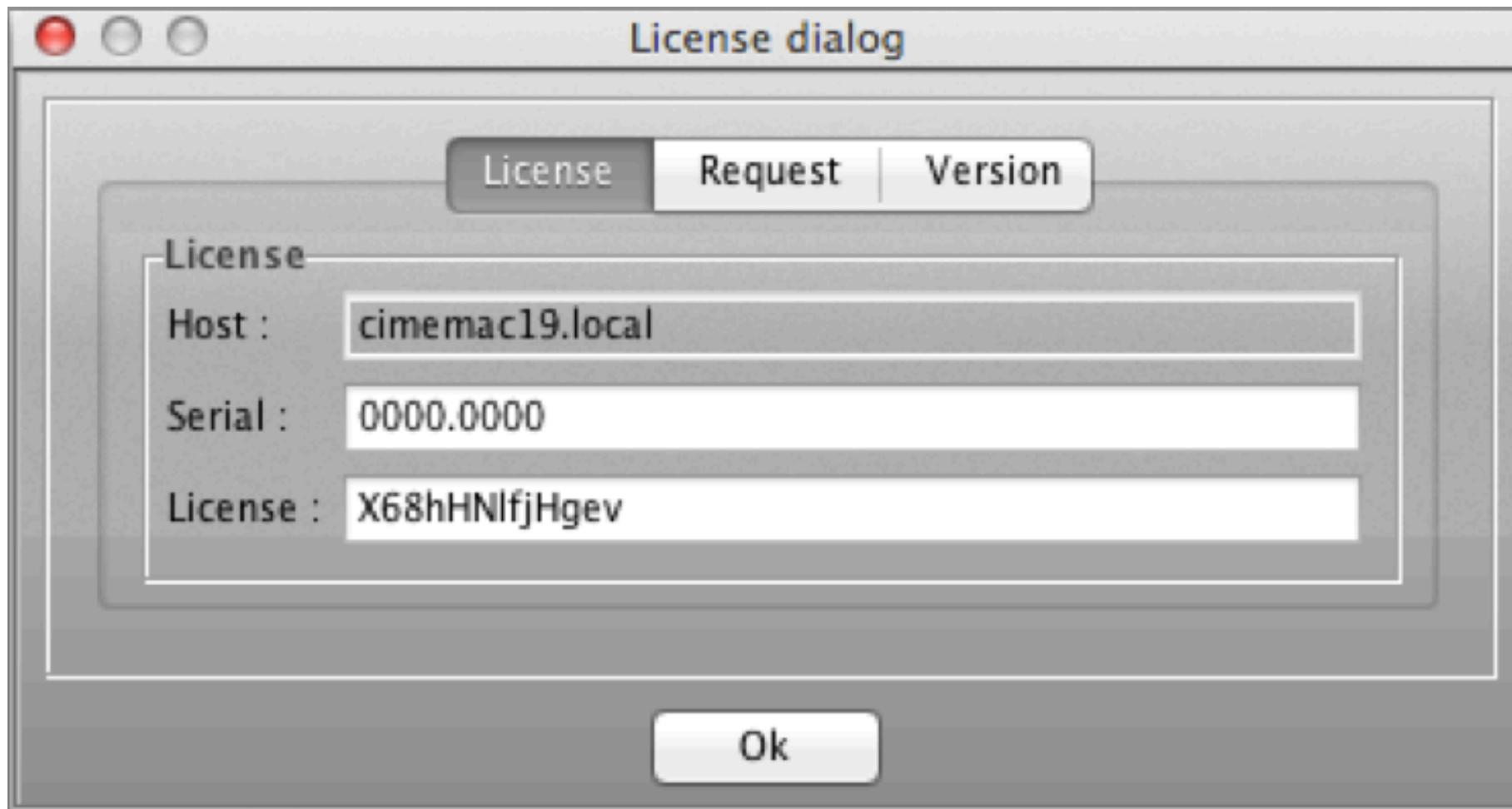
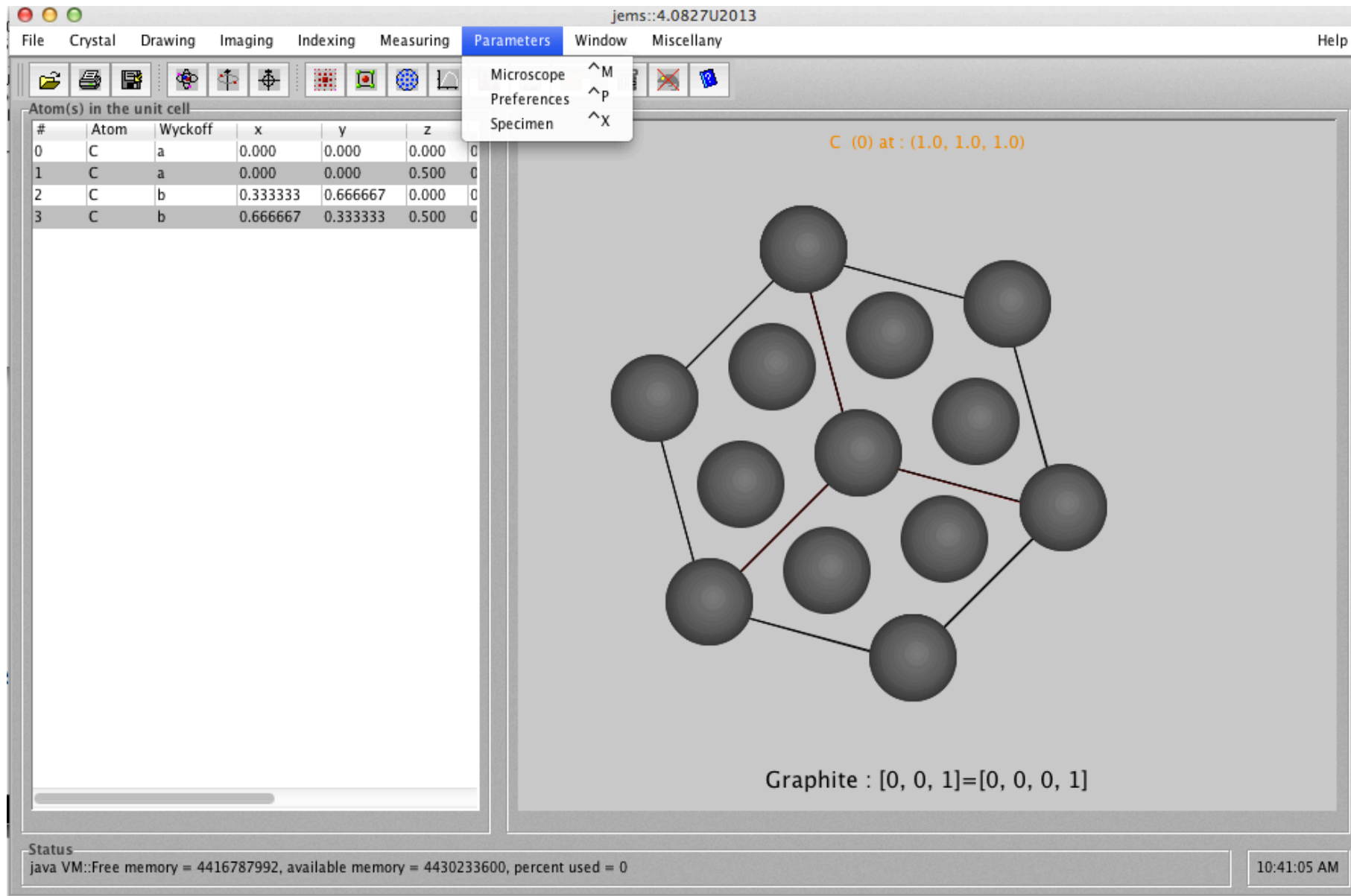


Figure: The license dialogue showing the **Host** name of the computer and **Serial** number.

The hostname and serial will be used to generate a license code.

# Preferences



The screenshot shows the jems software interface. The title bar reads "jems::4.0827U2013". The menu bar includes "File", "Crystal", "Drawing", "Imaging", "Indexing", "Measuring", "Parameters", "Window", "Miscellany", and "Help". The "Parameters" menu is open, showing "Microscope", "Preferences", and "Specimen". The "Preferences" option is highlighted. The main window displays a 3D ball-and-stick model of a graphite unit cell. The atoms are represented by dark gray spheres, and the bonds are black lines. The text "C (0) at : (1.0, 1.0, 1.0)" is visible above the model. Below the model, the text "Graphite : [0, 0, 1]=[0, 0, 0, 1]" is displayed. On the left side, there is a table titled "Atom(s) in the unit cell" with the following data:

#	Atom	Wyckoff	x	y	z
0	C	a	0.000	0.000	0.000
1	C	a	0.000	0.000	0.500
2	C	b	0.333333	0.666667	0.000
3	C	b	0.666667	0.333333	0.500

The status bar at the bottom shows "Status" and "java VM::Free memory = 4416787992, available memory = 4430233600, percent used = 0". The time "10:41:05 AM" is displayed in the bottom right corner.

Figure: Parameters → Preferences menu item allows to set default values of many jems parameters.

# Default crystal

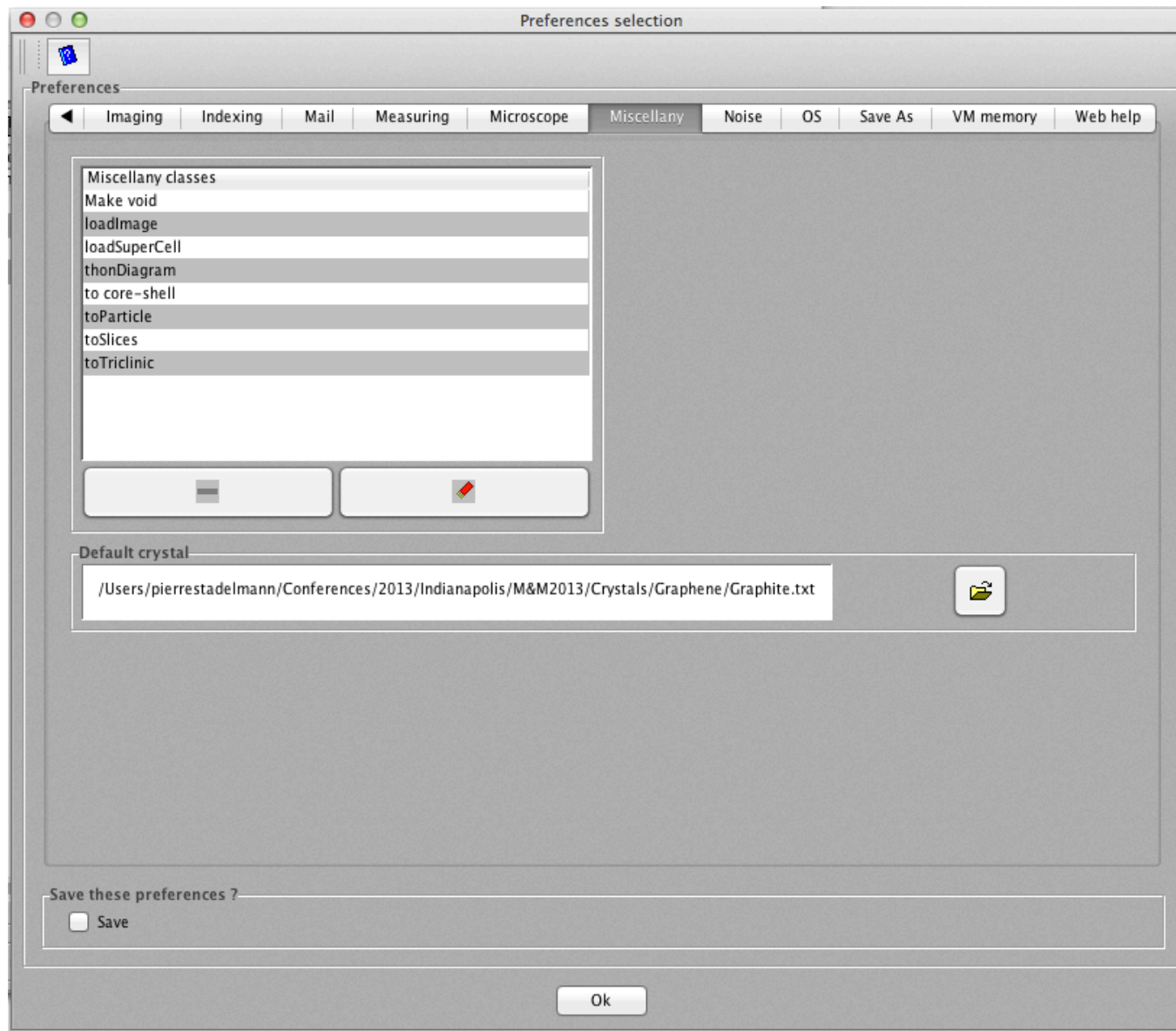


Figure: The default crystal is selecting when jems is started.

# Default crystal

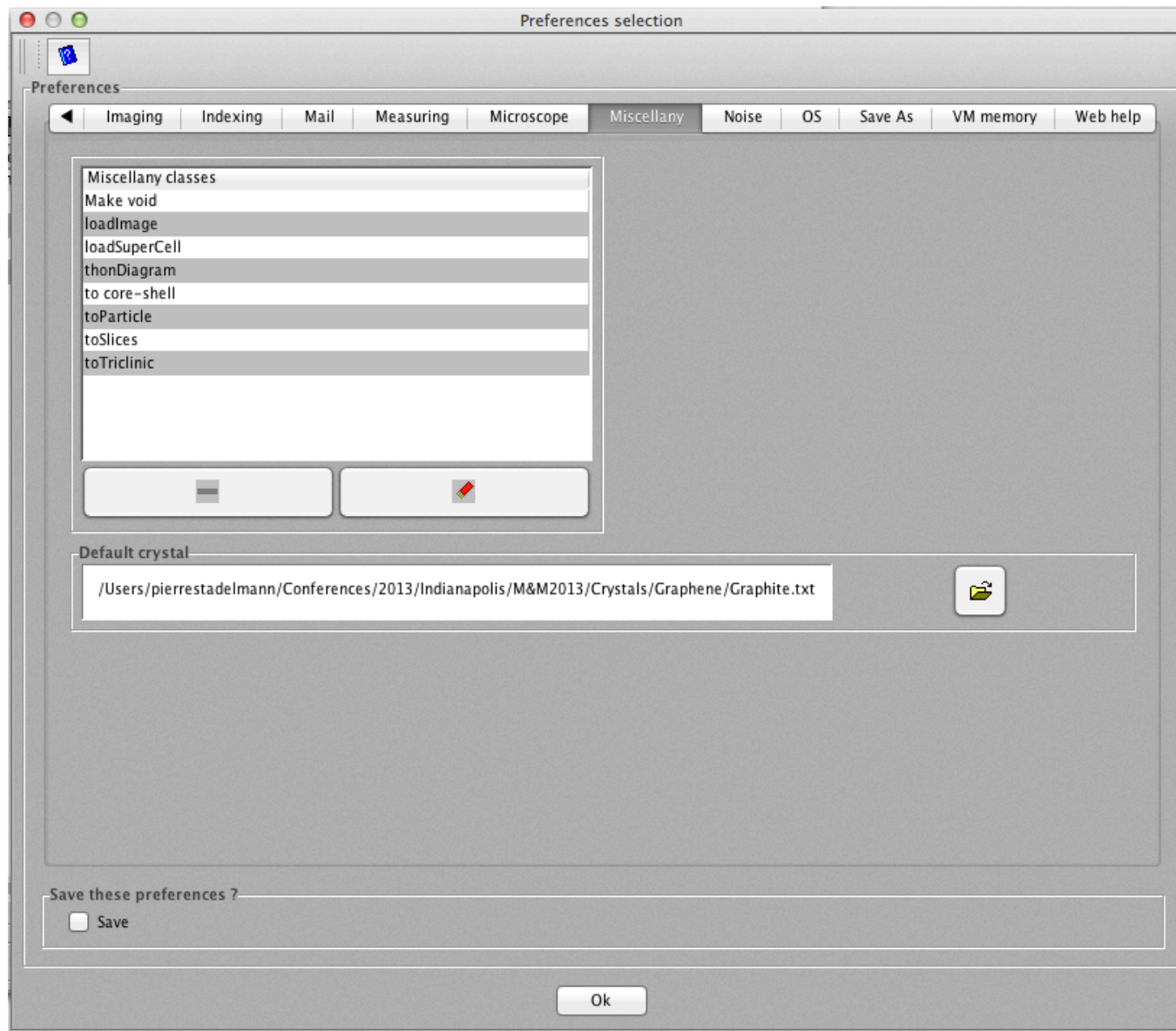


Figure: The default crystal is selecting when jems is started.



# Selecting Si

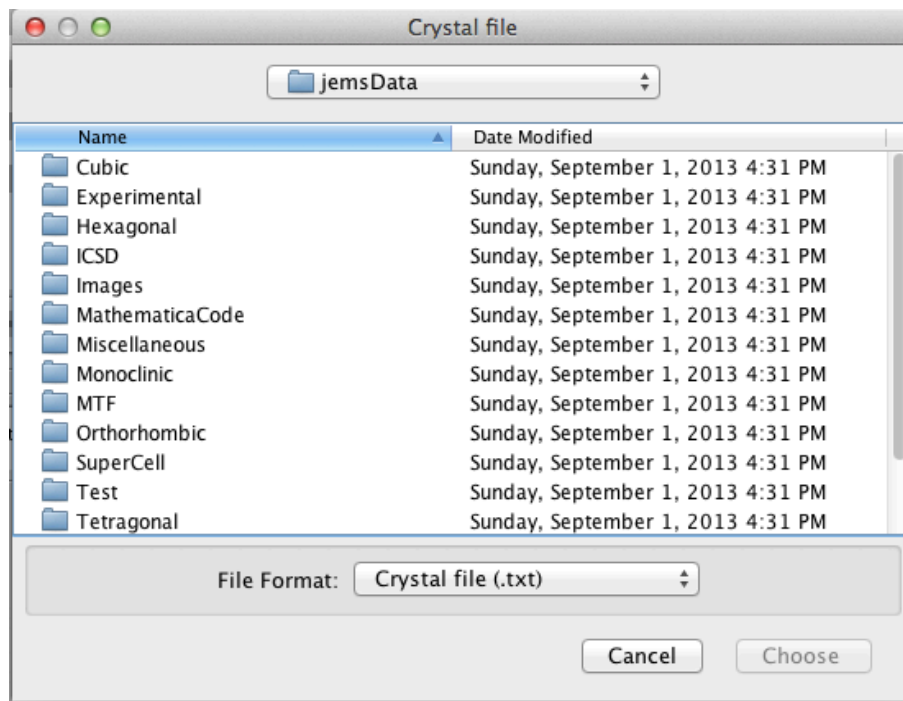


Figure: Crystal files are organized by crystal system.

Selected the Si crystal,

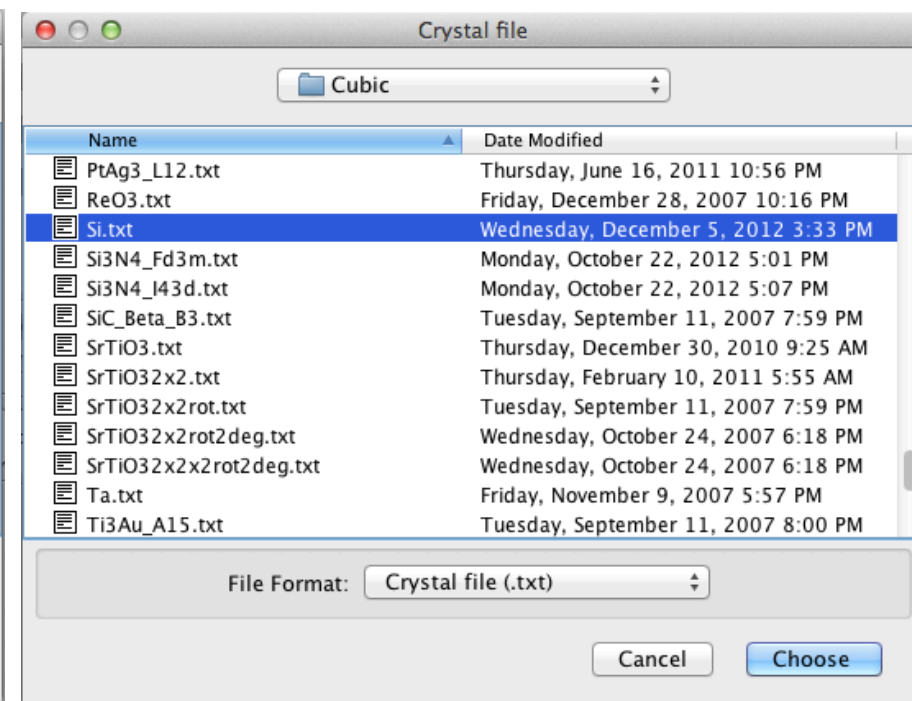


Figure: Si crystal file.

# Saving preferences

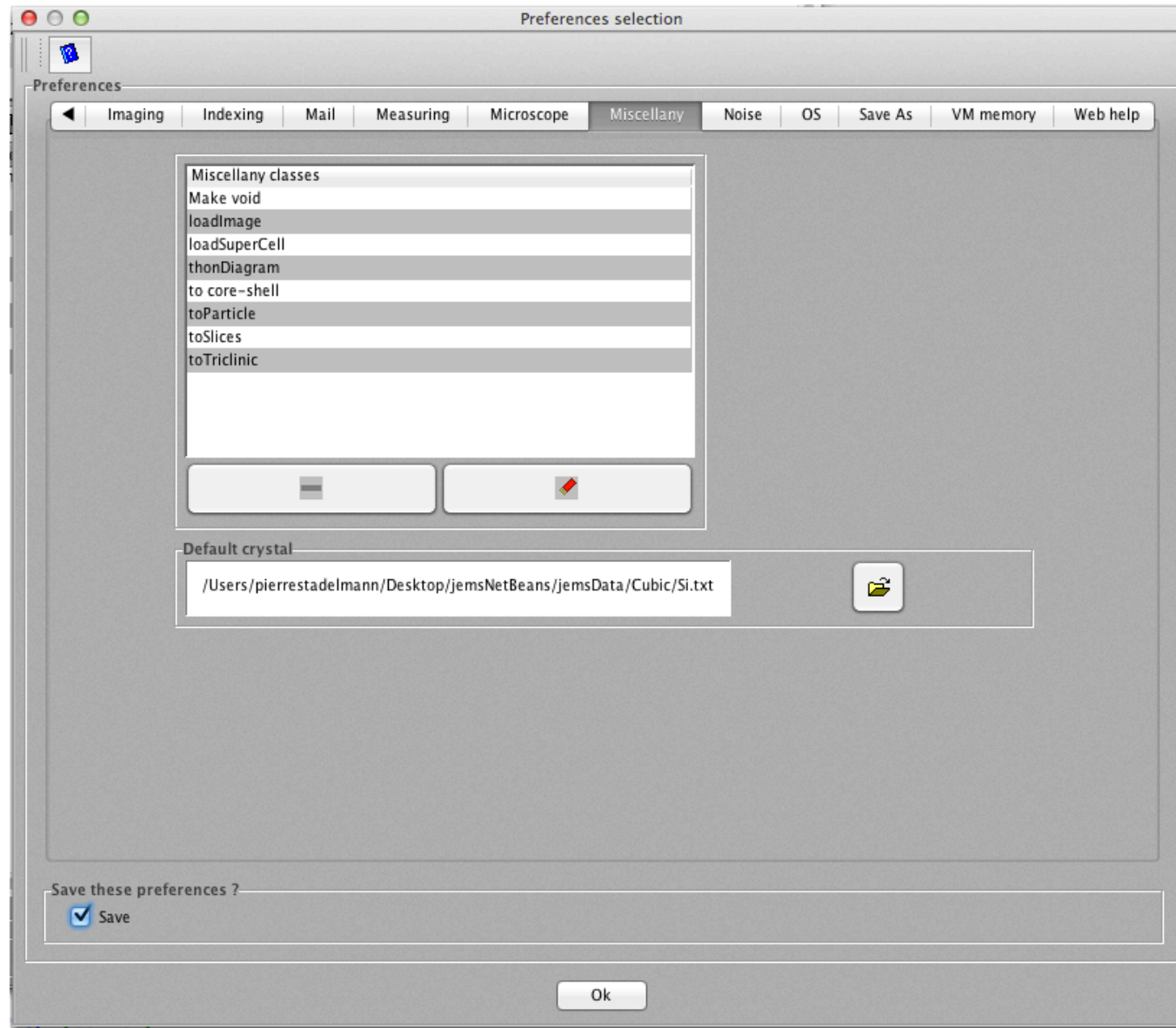


Figure: Cross the **Save** check box in order to save your preferences.

# USBKey documentation folder

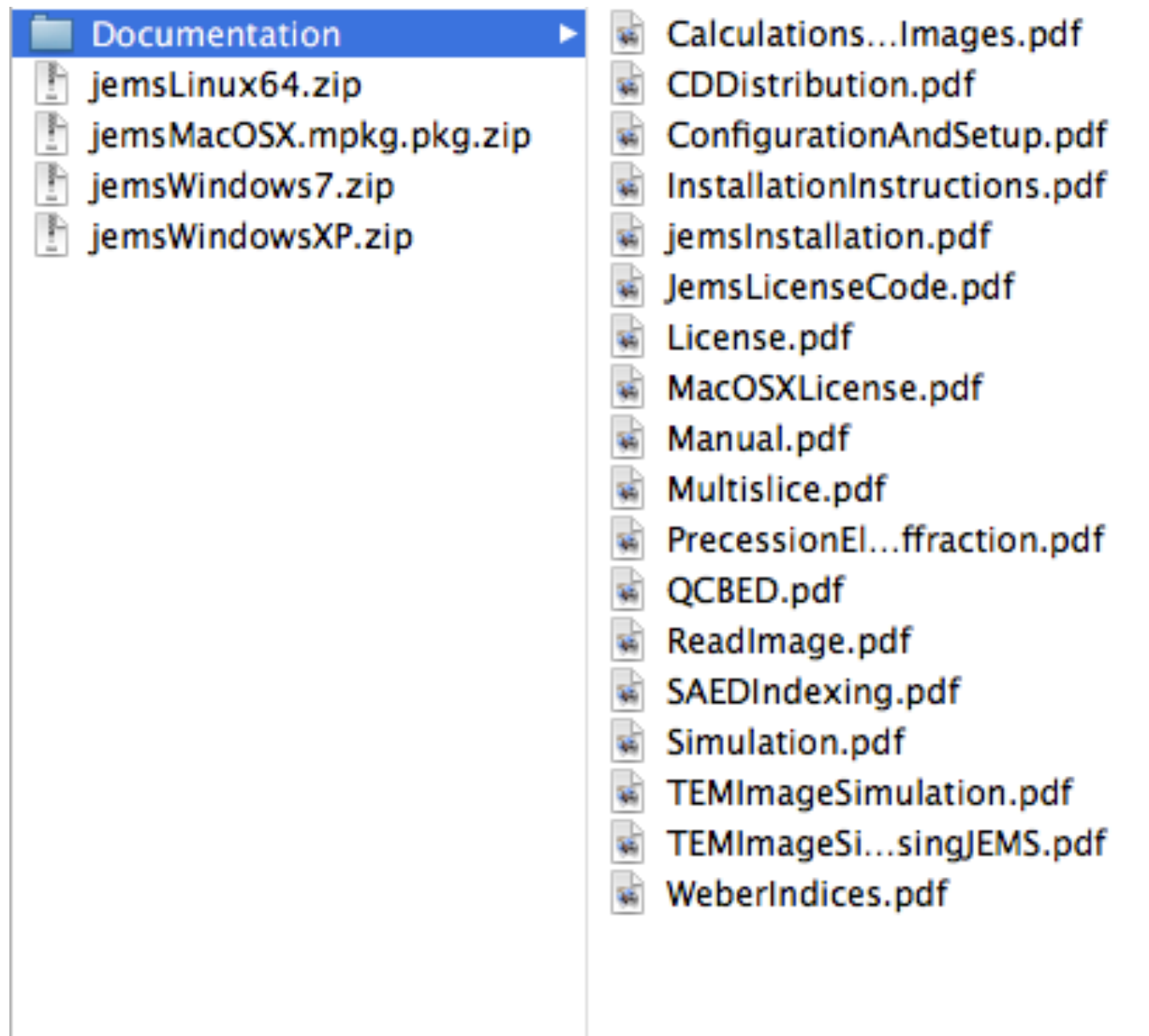


Figure: **Documentation** folder contains .pdf files explaining how to perform simulations using jems.

- ▶ Defining a new crystal and checking it.
- ▶ Structure factors and powder pattern, comparison with X-ray or neutron patterns.
- ▶ Setting a  $[uvw]$  crystal orientation and microscope parameters.
- ▶ SAED kinematical and dynamical diffraction patterns:
  - ▶ HOLZ lines.
  - ▶ Kikuchi lines.
- ▶ CBED and LACBED.
- ▶ PED (precession electron diffraction).
- ▶ HRTEM image simulation:
  - ▶ Bloch waves approach.
  - ▶ Multislice approach.
- ▶ Measuring CCD MTF.
- ▶ HAADF.
- ▶ ....

