jems preferences selection

Pierre Stadelmann Obere Lomattenstrasse 33 CH-3906 Saas-Fee Switzerland jems.stadelmann@gmail.com

July 11, 2014

Contents

1	Atom tab	3
2	Color tab	3
3	Contour tab	4
4	Debug tab	4
5	Display tab	5
6	Font tab	6
7	Imaging tab	7
8	Indexing tab	8
9	Mail tab	9
10	Measuring tab	9
11	Microscope tab	10
12	Miscellany tab	10

13 Noise tab	11
14 OS tab	11
15 Save As tab	12
16 VM memory tab	12
17 Web help tab	13

1 Atom tab



Figure 1: Atom tab: atom color selection. Figure 2: Color tab: text & panel background color selection.

The Atom color tab sets the atom $colors^1$.

2 Color tab

The Color tab sets text, drawing and images background colors.

¹Note that a tool tip text is attached to every control of the **Preferences dialogue**.

3 Contour tab

Atom	Color	Contour	Debug	Display	Font	Imaging	Indexing	Mail	Measuring	Microscope	Atom	Color	Contour	Debug	Display	Font Imagin	ng Indexin;	Mail	Measuring	Microscope	
					Leve	ls number						Debu	g options Blochwave	- CTF		Debug (simple	e) 🗆 Debug	(extended)	Finalize		
						-							Fit	C For	nat	Graphics	HAAD	F	Imaging		
						- 80							Indexing Printing	 Keyl Spo 	board ce-group	 Memory Table 	 Mouse Threa 	d	 Multislice Timing 		
						- 40							Zone axis								
						- 20						Final	izer categor Box	γ O Component	 Control 	 Crystal 	O Dialog	 Image 	 Indexing 		
													Manager Shape3D	 Math Selector 	 Miscellan Table 	y Object O Thread	 Other XRay 	 Panel 	 Shape 		
					1	2						Num	ber of cpu's	(core's)							
													1	0 2	• 4	O 6	• 8	0 12	0 16		
					Con	tour color							24	0 32	0 48	0 64	0 128	0 256	0 512		
												CIF	reading / En	ror logging / M	ulti-threading						
													CLP space-gr	oup		U E	rnor logging				
													Intensity su	m check		N 1	ava VM multi-th	reading			
Save these	preferenc	es ?									Save the	se preferen	ces ?								
Save												ve									
					C	Ok										Ok					

Figure 3: Contour tab: contour plot color Figure 4: Debug tab: debug, finaliser and and levels number selection. multithreading options.

The **Contour** tab sets the colour of the contour plots and the number of contour levels.

4 Debug tab

The **Debug** tag allows to debug jems operations (**Debug options**), to check that memory is released when dialogues and frames are close (**Finalizer category**), to set the number of available cores (**Number of cpu's**) and to set a few more options concerning .cif files reading (**CIF space-group**), error reporting (**Error loving**) and setting of java VM (**java VM multi-threading**).

When using a i7 processor set the core's number to 8 (i7 allows 2 threads per core).

5 Display tab



Figure 5: Display tab: sets several display Figure 6: Font tab: font type and size selecoptions. tion.

The **Display** tab deals with the display of jems drawings. The **Unit cell** ... box defines conditions to display crystal structures with minimum resolution. The **Display options** set:

- 1. Alpha composite: transparency of drawings and images. Alpha composite is set using using the slider Alpha comp.
- 2. Default atom size: set the atom radius to a 50 pm default.
- 3. **Plot intensity**: plot the intensity of the reflections instead of the amplitude as a function of crystal thickness.
- 4. Show hkl powder lines: when set displays the hkl powder lines on transfer function plots.
- 5. Show parallel projection: show a parallel projection of the structure in jems main window.
- 6. White background: plots drawing on a white background.

The **Q** max ... set of controls places a limit on the powder lines displays.

6 Font tab

The **Font** tab allows to select a given font and size. The number of available fonts depends on the operating system (OS).

7 Imaging tab

2 Preferences	D Preferences
Atom Color Contour Debug Display Font Imaging Indexing Mail Measuring Microscope 🕨	Atom Color Contour Debug Display Font Imaging Indexing Mail Measuring Microscope 🕨
Bioge stripe / montage Maximum abservations ander Show stripe Show montage	Digital micrographs Pixel size / mm : 0.07485022
Lowest beam amplitude considered for imaging 0 10-8 0 10-7 0 10-6 0 10-5 0 10-4 0 10-3 0 10-2	
Maximum dimension of EUE panels Maximum dimension of reduced images © 512 640 768 1024 1536 256 512 768 0 1536	
Maximum image dimension. ○ 256 ○ 384 ● 512 ● 640 ● 768 ● 896 ● 1024 ● 2048 ⊙ 4096	
Maximum mop dimension 0 512 0 640 0 768 0 896 0 1024 0 2048 0 4096 0 8192 0 16384	
Pixel size of high resolution images / rm. 0.001 0.002 0.004 0.005 0.006 0.008 0.01 0.02 0.04 0.05	
Petertial Interpolation O As is O Interpolate Subsomple O Bicubic	
Power spectrum O Legerithm scale O D01 O 1 O 10 100 1000 1000	
Jeve 30 Holography tob Check eton site ecoporcy Evole Evole Evole	
Give these preferences 7	Sove These preferences 7
Ok	OK

Figure 7: Imaging tab: image simulation op- Figure 8: Indexing tab: experimental pixel tions. size.

The **Imaging** tab groups controls and settings related to image simulation and graphical user interface (GUI). Typical settings are show in Figure 7. When using a large screen, the **Maximum dimension of GUI panels** can be increased to 1024 or more, allowing to calculate, for example, large CBED and LACBED patterns. The **Maximum image dimension** defines the maximum size of calculated images. The **Maximum map dimension** defines the maximum size of images map.

The **Pixel size of high resolution images / nm** sets the sampling used by the multislice calculation. A typical value is 0.001 nm.

The **Resize loaded images** set how experimental images are resized before being displayed. **Potential interpolation** sets the method employed to interpolate projected potential.

The Java 3D, Holography tab and Check atom site occupancy check boxes allow to display crystal structures using OpenGL, to simulate holograms and to check the occupancy of every atom site in a structure.

8 Indexing tab

The **Indexing** tab sets the experimental pixel size.

9 Mail tab

S .	Defenses
Atom Color Contour Debug Display Font Imaging Indexing Mail Measuring Microscope 🕨	Atom Color Contour Debug Display Font Imaging Indexing Mail Measuring Microscope 🕨
Mail settings	Measurement option(s)
SMTP server : mail.epfl.ch	Thickness All BW's
From : pierre.stadelmann@epfl.ch	
Te : pierre.stadelmann@epfl.ch	
Enable mail	
Save these preferences 7	Save these preferences ?
Save	Sove
Ok	(k)

Figure 9: Mail tab: e-mail settings.

Figure 10: Measuring tab: QCBED profile option.

The **Mail** tab defines the out going mail server, your e-mail address and the e-mail address of the recipient. The **Enable mail** check box is used to mail newly created crystal files.

10 Measuring tab

The **Measuring** tab defines how QCBED thickness profiles are calculated. QCBED uses the Bloch wave method and a limited number of reflections can be included in the calculations.

11 Microscope tab



Figure 11: Microscope tab: defines the de-Figure 12: Miscellany tab: defines the default microscope. fault crystal.

The **Microscope** tab sets the microscope characteristics² and the range of the contrast transfer function (CTF) plots. Note that 20 nm^{-1} corresponds to 0.5 Ångström.

12 Miscellany tab

The **Miscellany** tab sets primarily the default crystal, i.e. the crystal that is loaded at start time.

 $^{^2 {\}rm Microscopes}$ not defined here can be created using the Microscope dialogue.

13 Noise tab



Figure 13: Noise tab: characteristics of the Figure 14: OS tab: look and feel of graphical noise that can be added to simulated images. user interface.

The **Noise** tab defines the type and amplitude of the noise that can be added to simulated images.

14 OS tab

The **OS** tab sets the *Look and Feel* of the user interface and allows to activate a few type of windows events (when not taking into account by the OS).

15 Save As tab



Figure 15: Save As tab: format of saved im- Figure 16: VM memory tab: java VM memages. ory settings.

The **Save As** tab defines in which format images or drawings must be saved³.

16 VM memory tab

The **VM memory** tab defines the size of java VM memory allocated at start time, the maximum size of java VM memory and the stack size.

³The jems format is not always available.

17 Web help tab



Figure 17: Web help tab: url of help files.

The **Web help** tab defines the url of jems help files and the url web site where more info is available.