Installation of Elle/VPFFT processes and utilities

Before starting simulations or even preparing *.elle files, you will have to install Elle and the required codes that are not included in the Elle release yet (referring to the available Elle release in March, 2017). The first and most important step is to install Elle itself. This instructions are optimized for Ubuntu 14.04 or for other Debian-based Linux distributions apart from Ubuntu 16 or newer. It is recommended that you follow these instructions reading a PDF file on your computer, as you may want to copy and paste the commands instead of typing them. You can find a similar instruction on www.elle.ws.

Step 1:

Install the following packages in the terminal

Open a terminal from anywhere and type this as one command line:

sudo apt-get install gfortran gcc mesa-common-dev libgl1-mesa-dev libglu1-mesa-dev libgtk2.0-0 zlibc zlib1g make build-essential xorg-dev libmotif4 libmotif-dev xutils-dev libgtk2.0-dev cvs xutils libx11-dev libXt-dev libxpm-dev x11proto-print-dev x11proto-xext-dev libxext-dev

Step 2:

Download wxwidgets (http://www.wxwidgets.org/)

Make sure NOT to download the latest version (3.xx), but the previous stable release (2.8.12). You can find it under Downloads -> Previous Stable Release 2.8.12 -> Source Code (wxAll ZIP version). Unzip, open in terminal and type:

./configure
make
sudo make install
sudo ldconfig

Now, the zip folder and the extracted folder may be deleted

Step 3:

Download Elle by opening the terminal and typing:

cvs -z3 -d:pserver:anonymous@elle.cvs.sourceforge.net:/cvsroot/elle co -P elle

Step 4:

Copy the *elle* folder to *home/your_username/programs/*

Change “your_username” according to your user-name. It is highly recommended that you use this directory. You can use a different directory, of course, but all codes in this tutorial are optimized for installation into in this directory. Changing the directory means a lot of additional steps that are not explained here.

Step 5:

Add necessary changes to Elle main-codes and install Elle

Open *home/your_username/programs/* and find the data in *FS_ElleChanges.* Copy the files found in *FS_ElleChanges/basecode* to elle/elle/basecode (replaces some old files). Replace the folders "*tidy"* and *"view"* in *elle/elle/utilities* with the folders found in *FS_ElleChanges/utilities.*

Open *home/your_username/programs/elle/elle* in a terminal and type "*chmod +x ./install.sh*", afterwards run the installation bash script typing:

./install.sh wx

Please wait, you will get some warnings, but hopefully no errors. Type *make clean* when installation is finished.

Step 6:

Add Elle path to .bashrc

Open the file .bashrc from your home directory (e.g. type *gedit ~/.bashrc*) and add the following lines at the bottom (replace *your_username* with the correct user-name). Afterwards save and close the file.

export PATH=$PATH:/home/your_username/programs/elle/elle/binwx
export LD_LIBRARY_PATH=/lib:/usr/lib:/usr/local/lib
export ELLEPATH=/home/your_username/programs/elle/elle/binwx
export BASILPATH=/home/your_username/programs/basil/bin
export PATH=${PATH}:$ELLEPATH:$BASILPATH:

Step 7:

Checking if Elle is installed

Now close all terminal windows, open a new terminal and type *showelle*. If the graphical user interface "*showelle*" is opening, you successfully installed Elle, congratulations. You can add "*showelle*" as an "open with" option, to quickly visualise Elle files. Find the instructions under www.elle.ws → Installation (step 8).

Step 8:

Install the remaining Elle/VPFFT codes

To run an Elle/VPFFT simulation, you need to install additional Elle modules. All of these modules and codes are found in *FS_Codes* (digital appendix). This folder contains all recrystallisation and VPFFT codes and some other utilities that are helpful to pre- or post-process the simulations. Copy this folder to *home/your_username/programs/elle/elle*, you can rename it, if you like. Open a terminal from *elle/elle/FS_Codes* and type:

chmod +x FS_install.sh

FS_install.sh

Wait until the installation is finished. You may see some warnings again, but hopefully no errors.