Step by Step to Complete CP Simulation

This manual aims to give a detailed guide for the fresh hands in Dr. Lian's group to perform CP (Crystal Plasticity) simulation dealing with the influence of strain rates and orientations by the means of parameter fitting.

Four parts are in this tutorial material including the parameter edition, the usage of Putty, plotting load-displacement curves as well as plotting pile-ups.

1. Edit the Parameters (Grain Orientation and Model Parameters)

1.1 Grain Orientation

1) Use Notepad to pen Grain Data

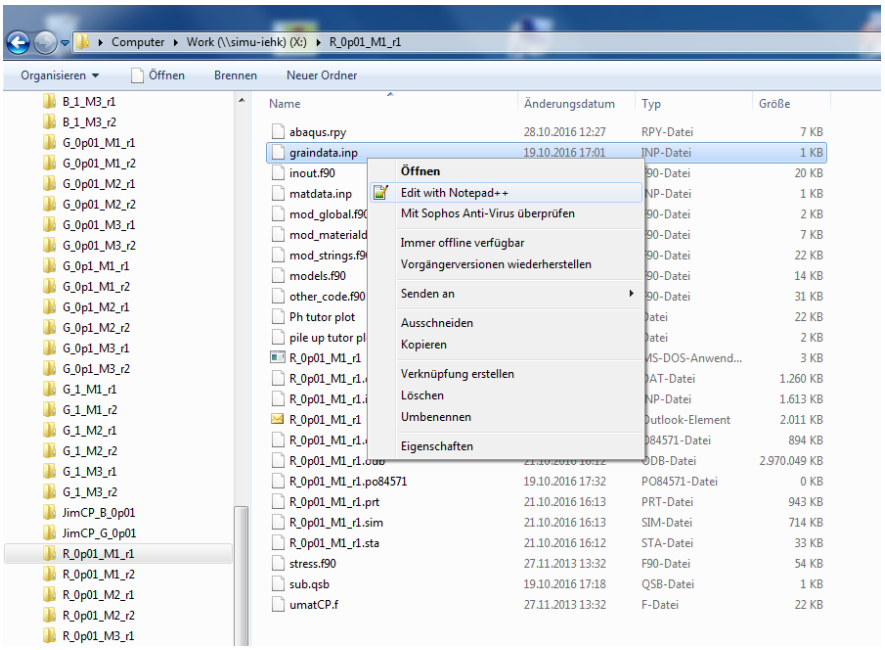


Fig. 1.1 open grain data to edit grain orientation

2) Edit Euler angles

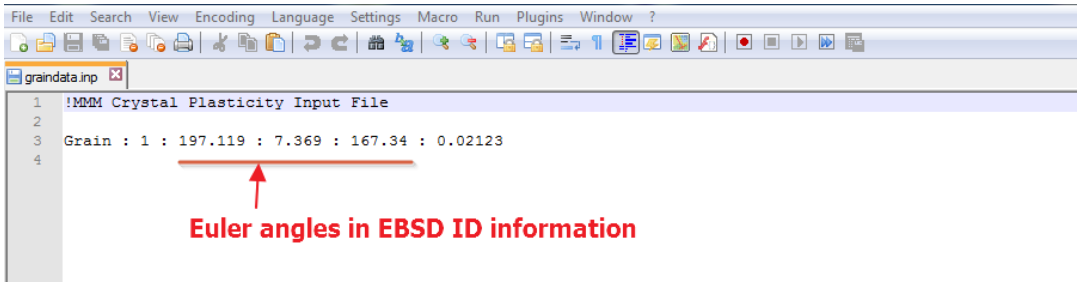


Fig. 1.2 change the three numbers marked according to the IQ map from EBSD package

These Euler angles are between 0~360°.

1.2 Model Parameters

There are 6 parameters to calibrate. These parameters may have different names as presented below. If the user has a different understanding about them, it is also acceptable.

τ_0: critical resolved shear stress (CRSS), in MPa

$\dot{\gamma}_0$: initial strain rate, in /s

$1/m$: m is strain rate sensitivity, in 1.

h_0: initial hardening slope, in MPa

τ_c^s:CRSS for cross hardening, in MPa

a: hardening exponent

Complete the following procedures to edit the simulation parameters above used for ABAQUS simulation.

1) Open matdata as below.

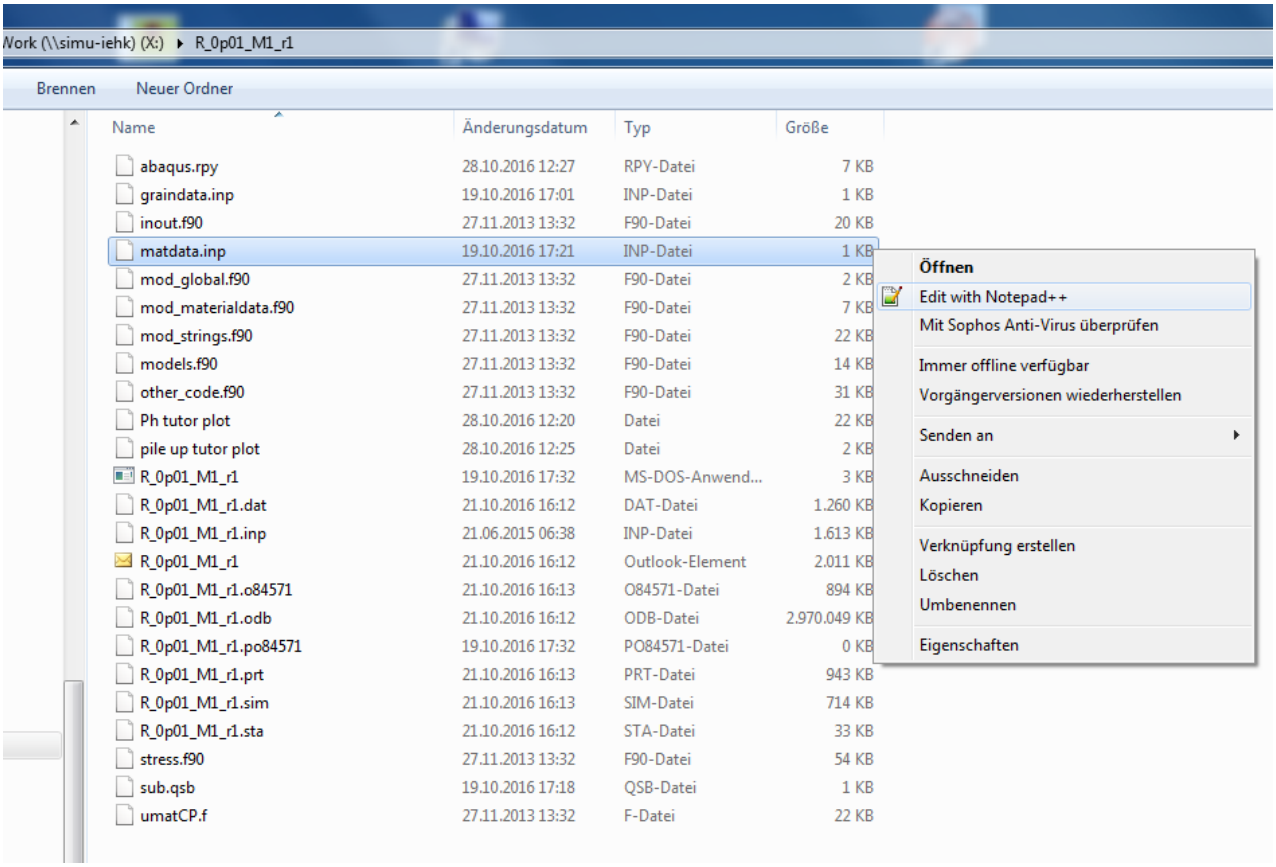


Fig. 1.3 open with Notepad

These parameters have different labels in matdata as shown below. **They are for BCC (ferrite simulation) mode**.

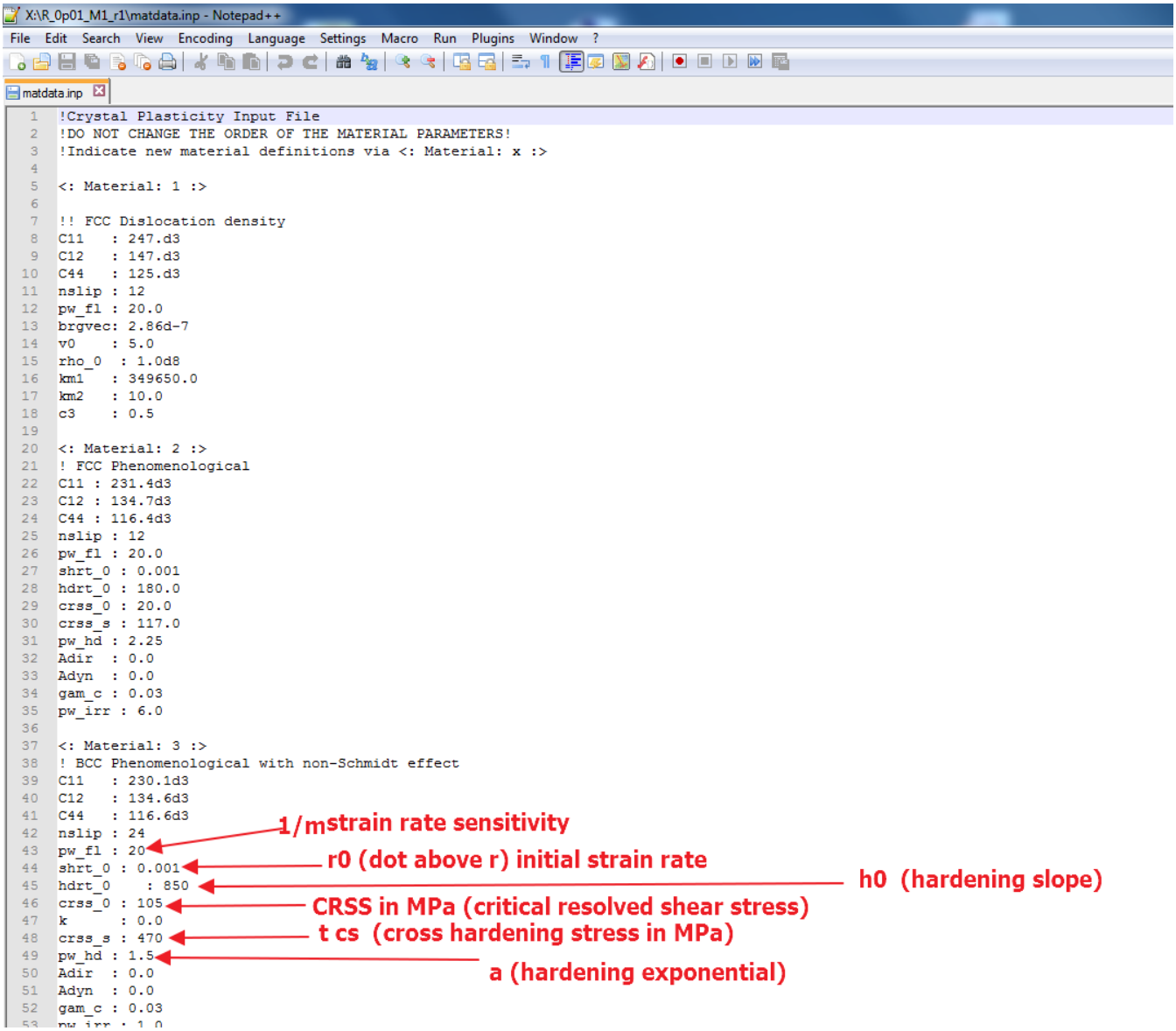


Fig. 1.4 edit the parameter in matdata then save this file

Edit them correspondingly and then save the edited version

There are 12 files in the folder to submit which are marked blue in Fig. 1.5.

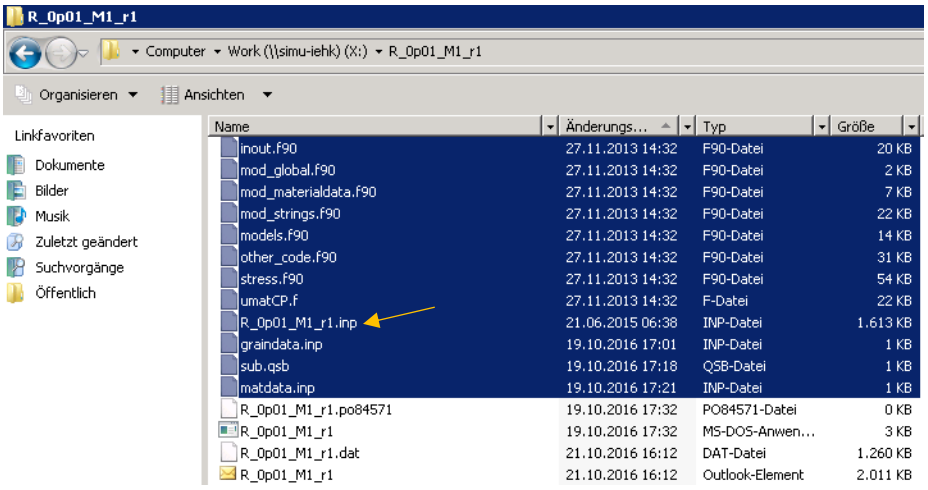


Fig. 1.5 Twelve files to submit in the folder in X disk

For the input files of different strain rates, the input file (.INP), as yellow arrow marked in Fig. 1.5, should be replaced. Here is the sample for 0.01/s (strain rate).

ABAQUS use the input files and the rest files of these 12 files including UMAT (user defined material), the codes etc. to carry on the simulation work simulation work.

3) Check the QSB file before the submitting

sub.qsb

```
#!/bin/sh
########################################
## Grid Engine QSB file
## Created by QSub Build 2015-02-26
## Date: 02.03.2015 11:40:30
########################################
#$ -N B_0p01_M1_r1
#$ -o /home_work/cpeng/B_0p01_M1_r1
#$ -j y
#$ -pe ncpus 1
#$ -hard -l h_vmem=8000M
#$ -hard -l ifort=true
#$ -hard -l h_rt=480:0:0
#$ -m e
#$ -m a
#$ -M Cheng.Peng@iehk.rwth-aachen.de
#$ -hard -l a_abq=true
module load abaqus
cd /home_work/cpeng/B_0p01_M1_r1
abaqus interactive job=B_0p01_M1_r1 input=B_0p01_M1_r1.inp memory=8000mb cpus=1 user=umatCP.f

```

Fig. 1.6 this is the recommanded method to organize a QSB file which is quite effective

2. Use Putty to Perform Simulation

Complete the following procedures to submit the simulation work.

1) Open Putty

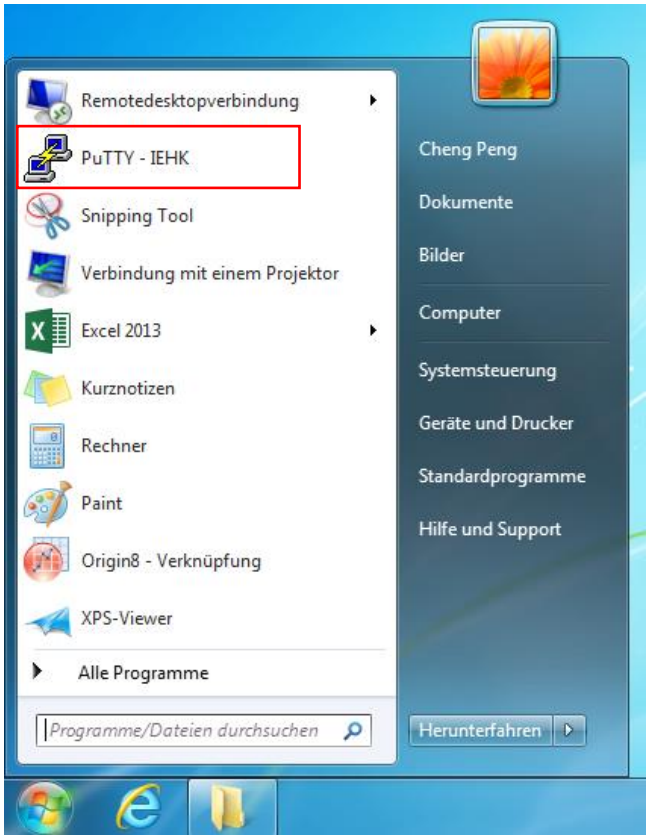


Fig. 2.1 click to start Putty

2) Put in “cluster-iehk” and press enter button, then click “open” button

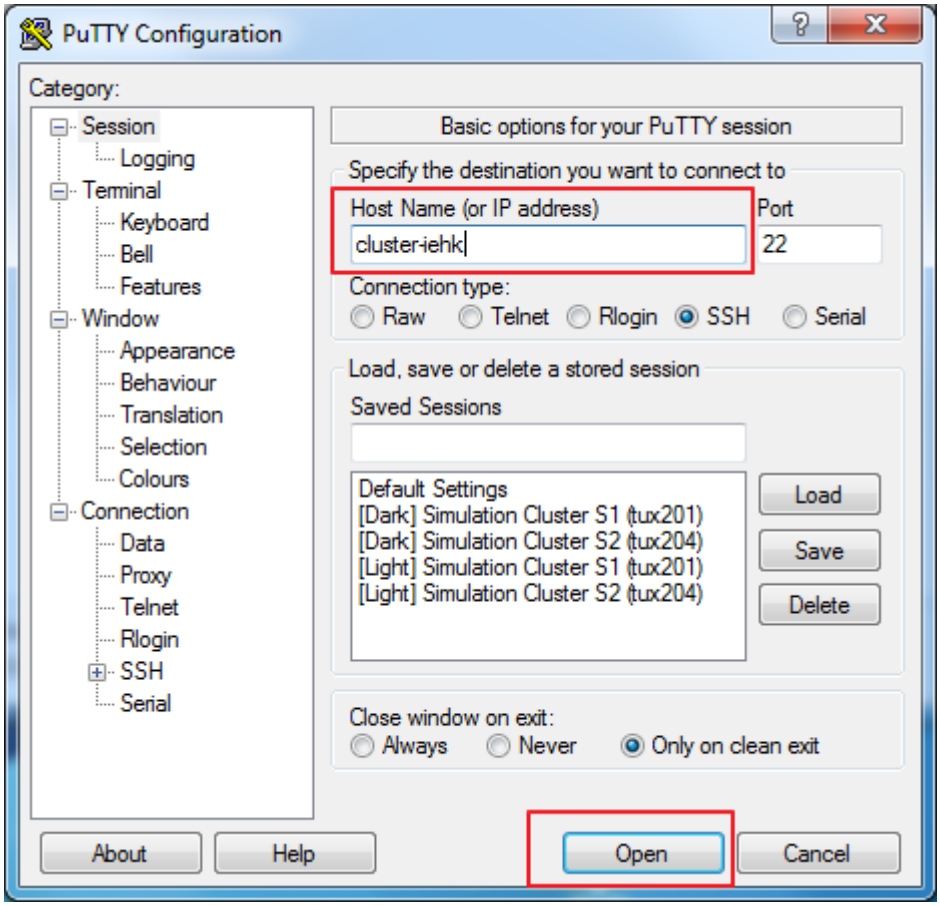


Fig. 2.2 start the DOS operation system

3) Log in with iehk ID

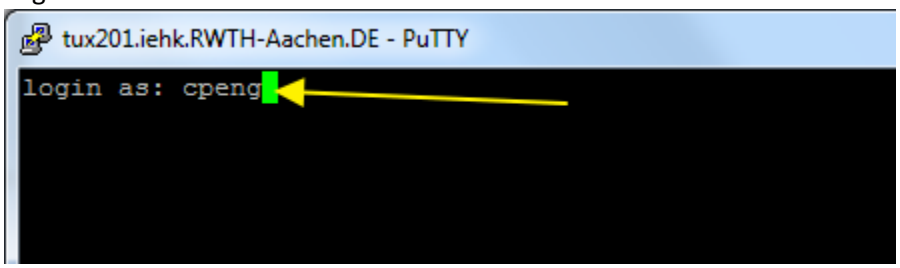


Fig. 2.3 Log in then press enter button

4) Type “cd $WORK” to go to the work space

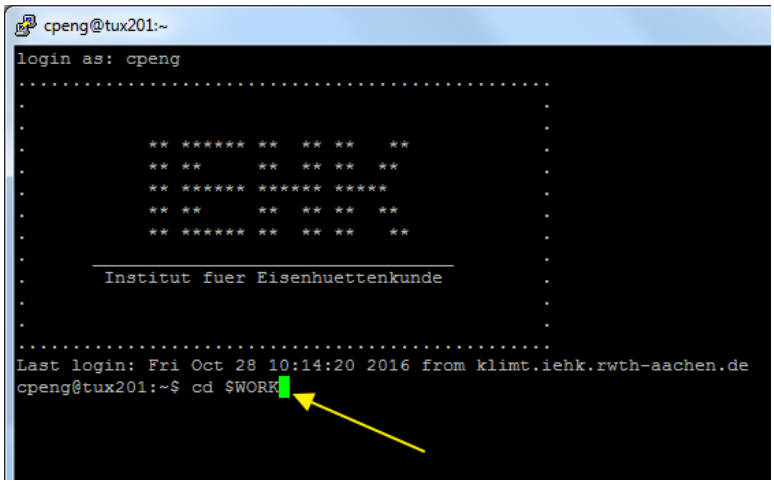


Fig. 2.4 there is a SPACE between d and $

5) Following content telling you that you are in your work space

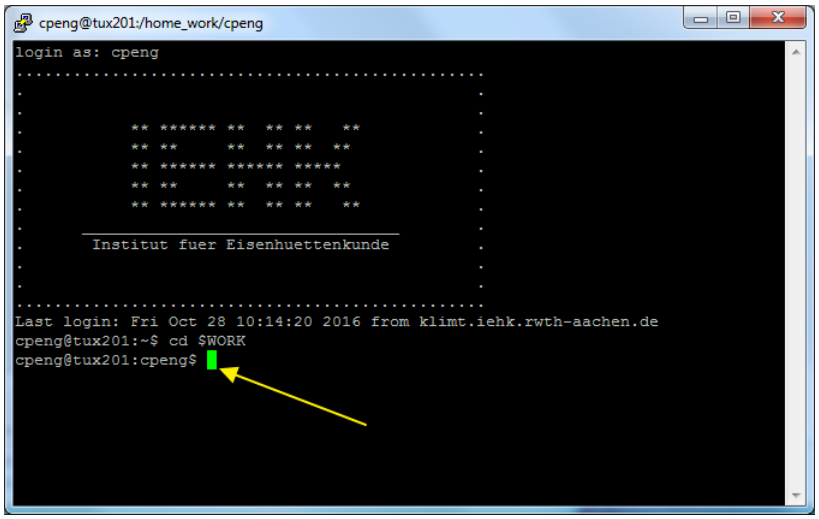


Fig. 2.5 in the work space of cpeng

6) Type “ls” to view the content of the folder i.e. the current work space

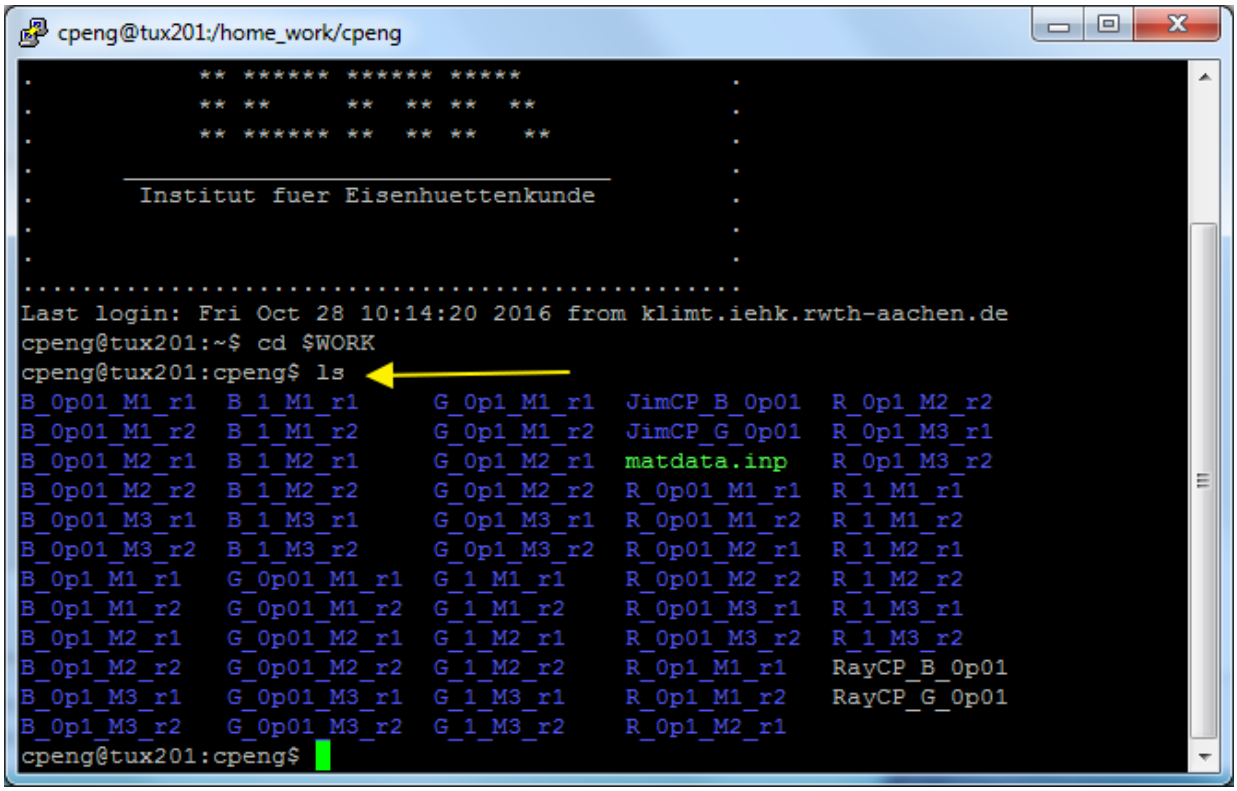


Fig. 2.6 the content of t he work space cpeng

7) Type “cd ” (a SPACE after cd), then double click “G_M2_r2” (the folder you’d like to open), the item is then died blue, after this, right click. DOS will copy the name of the item “G_M2_r2” after “cd ”.

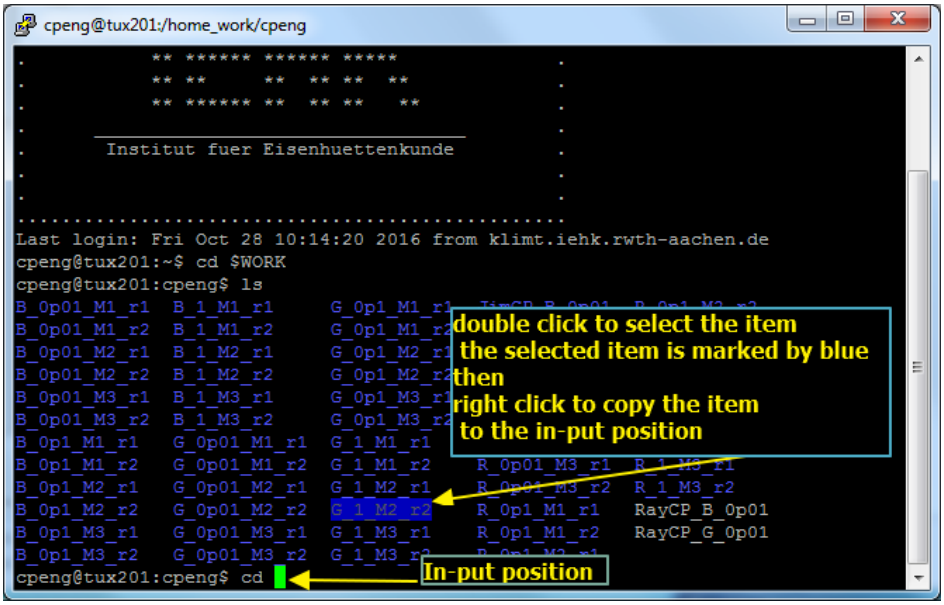


Fig. 2.7 open a folder in a fast way

8) The folder “G_M2_r2” is then open

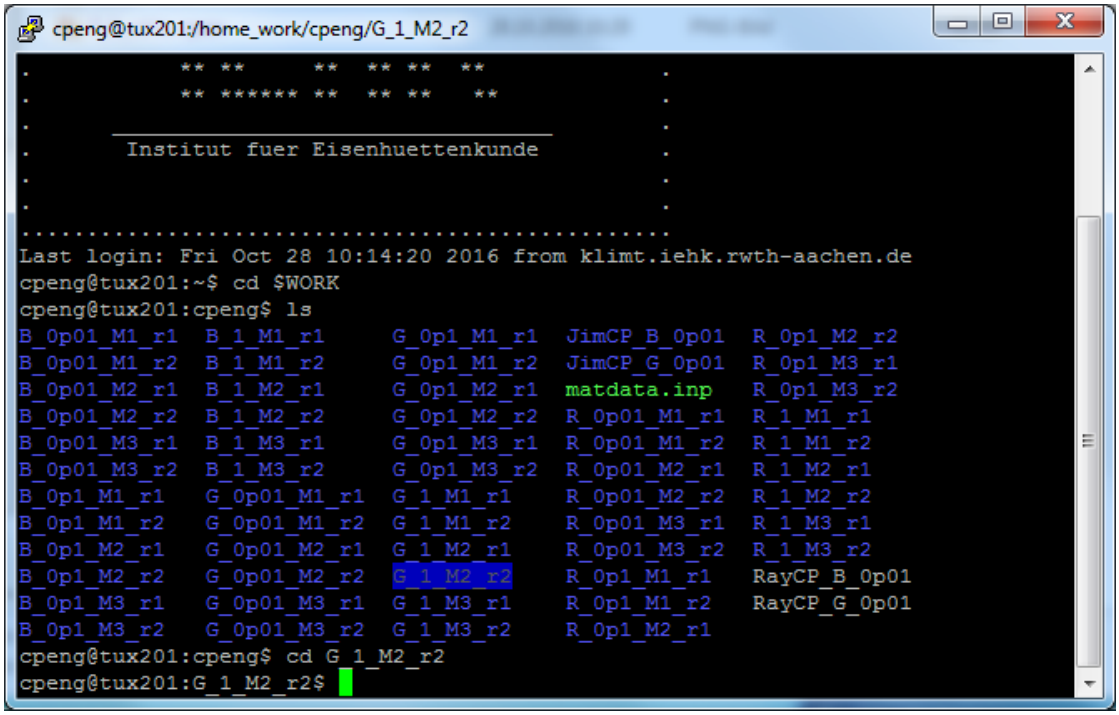
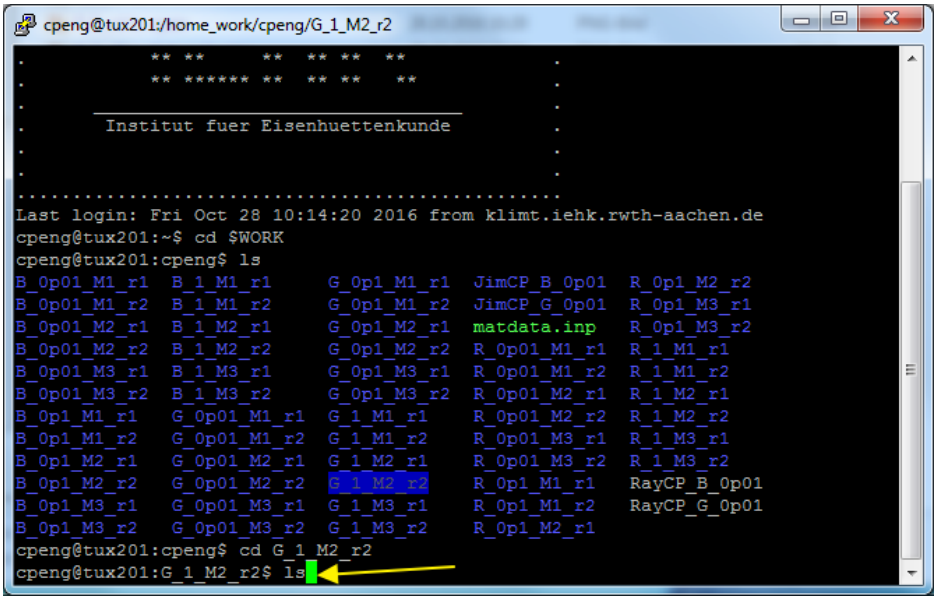
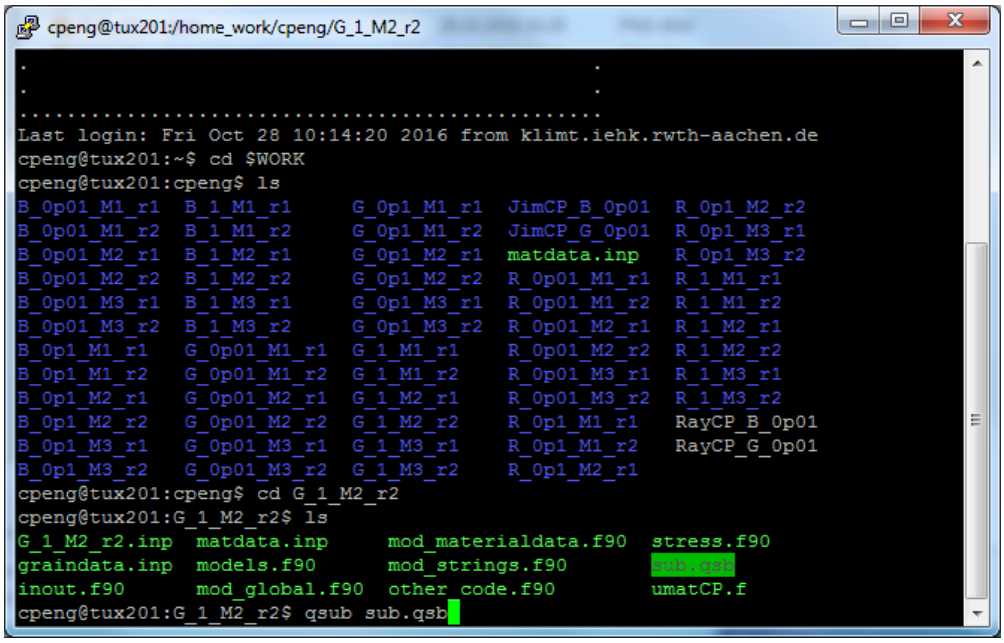


Fig. 2.8 open

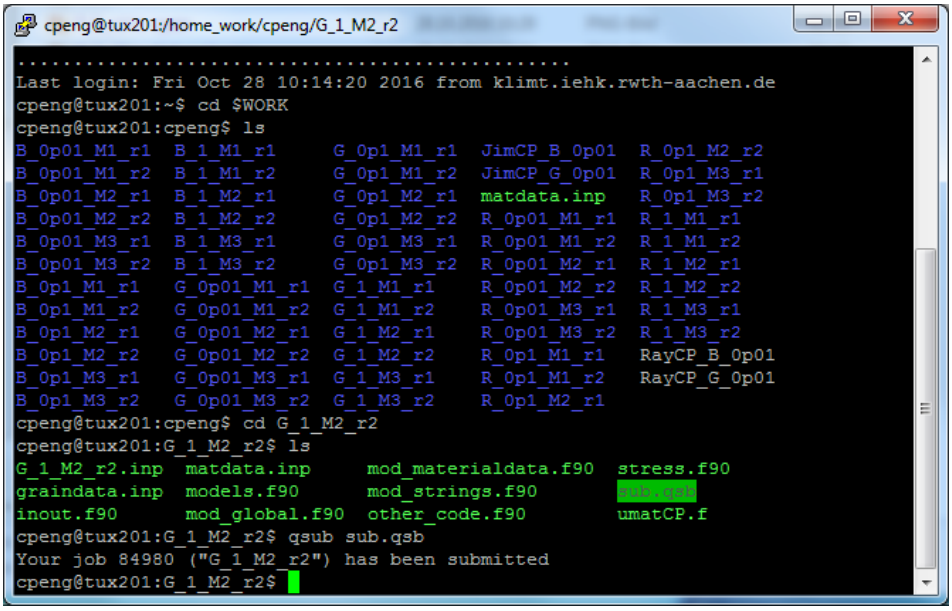
9) Type “ls” to view the content of “G_M2_r2”



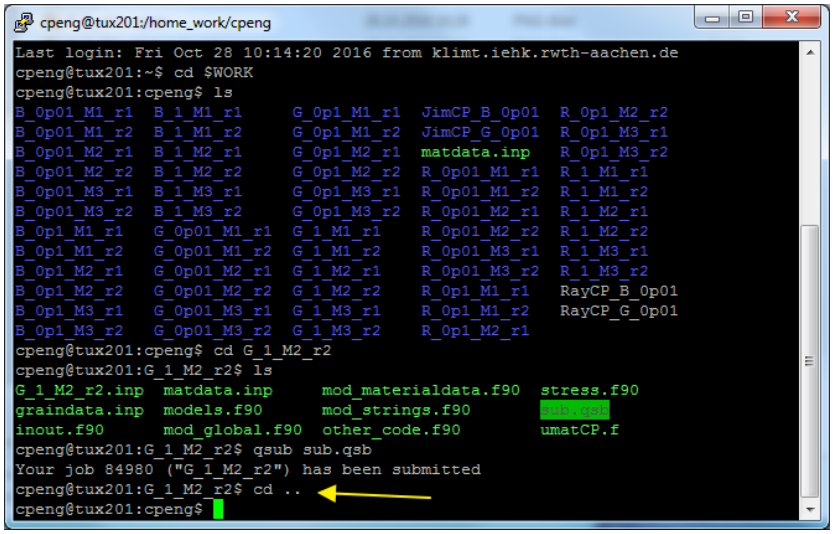
10) Type “qsub ” (a SPACE after b), then copy “” after “qsub ”, then press enter button.



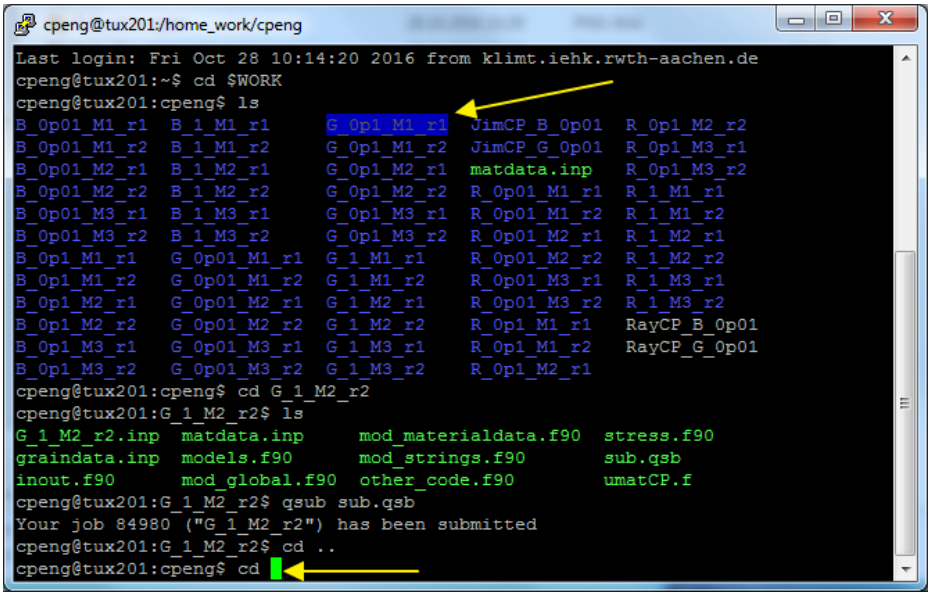
11) The work is submitted.



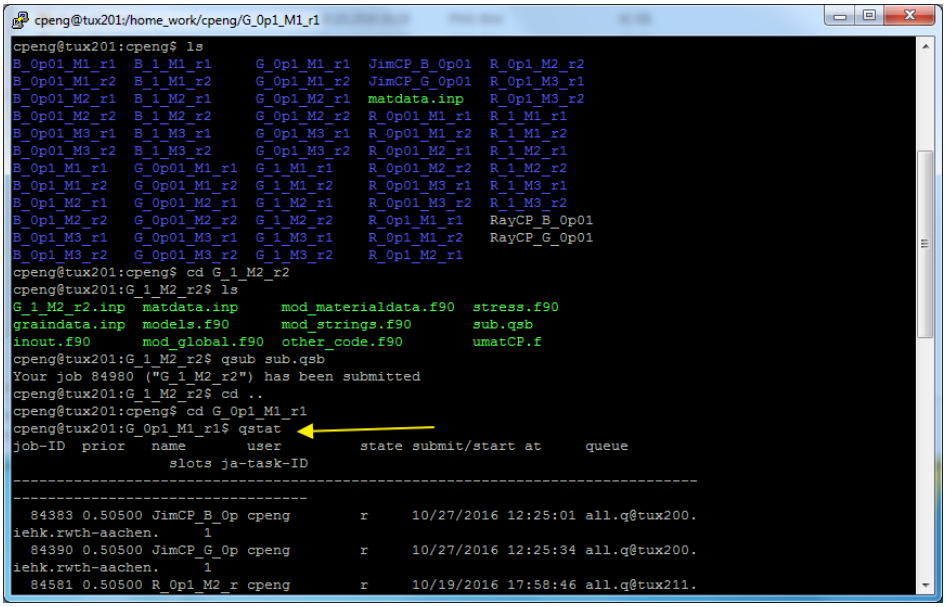
12) Type “cd ..” (a SPACE between d and .) to go back to the mother folder of the current folder i.e. the work space. In this way, you can open other folders in the work space or in the mother folder.



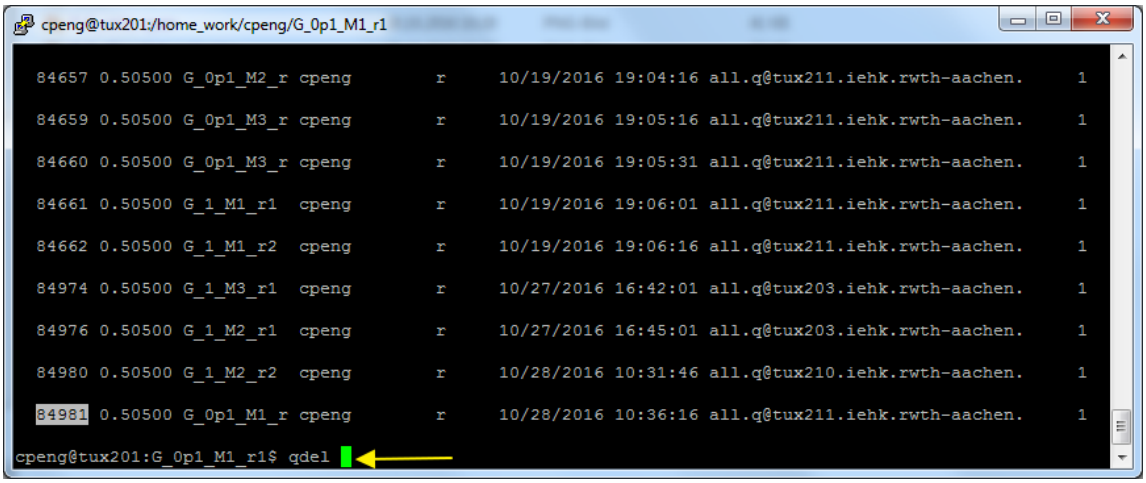
13) Type “cd ” to open e.g. “G_0p1_M1_r1” in the way as described since 7) in Fig. 2.7 above. Then submit and so on as described before to submit this work.



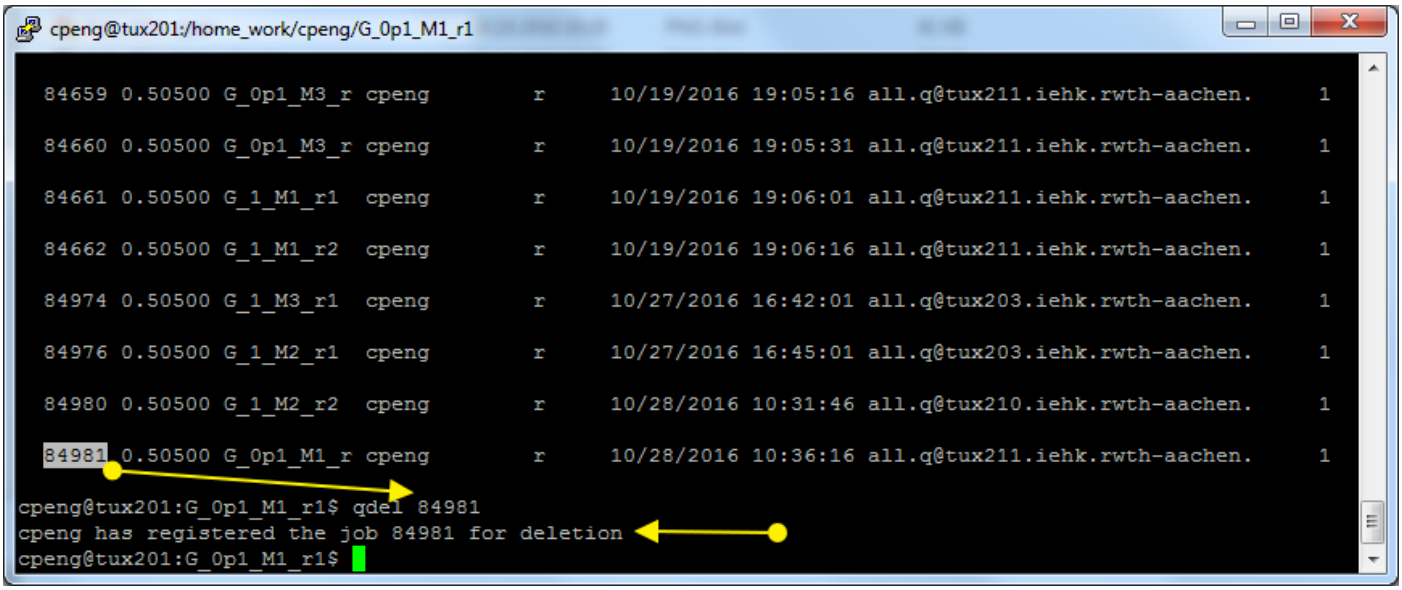
14) Type “qstat” to view the situation of the submitted work.



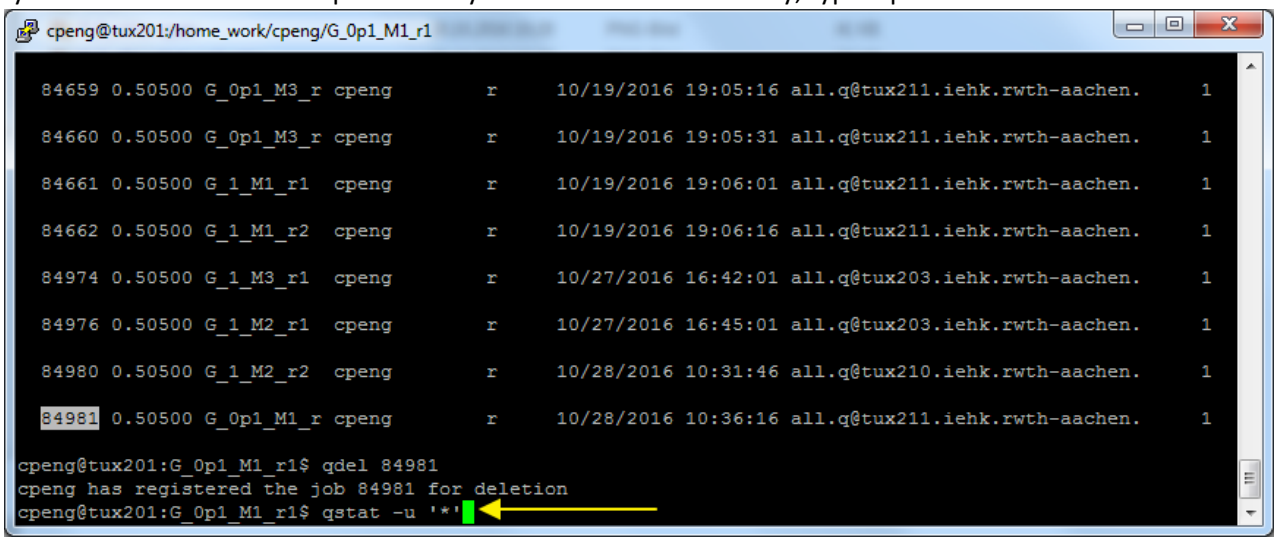
15) If you would like to stop the submitted work, type “qdel ” (a SPACE after l) and copy the work number e.g. 84981 of “G_0p1_M1_r1” submitted above, then press enter. This submitted work will be deleted.



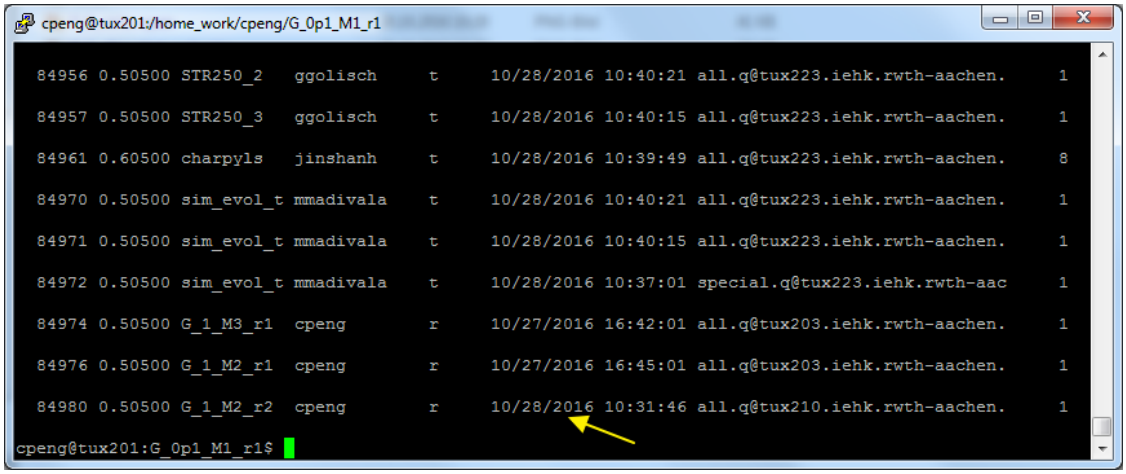
16) The work is deleted



17) If you would like to view the position of your work in the IEHK Putty, type “qstat –u ‘*’”



18) Your submitted work is presented then

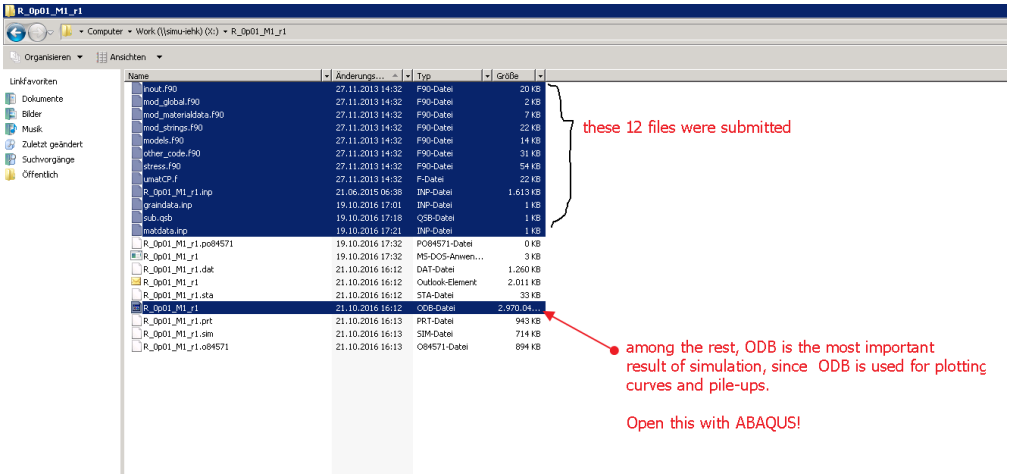


Forget about some skills in windows operation system, DOS is a whole new ball game.

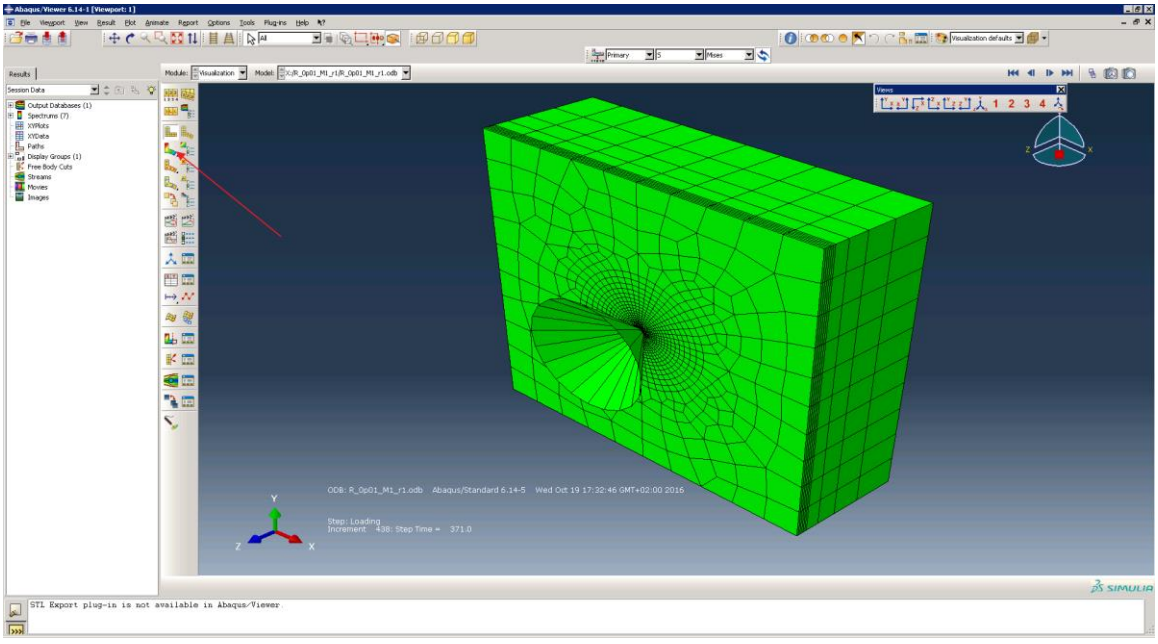
3. Plot Load-Displacement (P-h) Curves

Complete the following procedures to plot a load-displacement curve from the ODB data i.e. the completed simulation result.

1) Open the ODB with ABAQUS



2) After opening



3) Present the deformed shape to check whether the result is usable, because sometimes simulation provides useless result i.e. an ODB which could not present the deformed shape, even though it has taken much time to achieve this useless ODB. If it can deform, then open “creat XY data” by single click the button in Fig. 3.1 below.

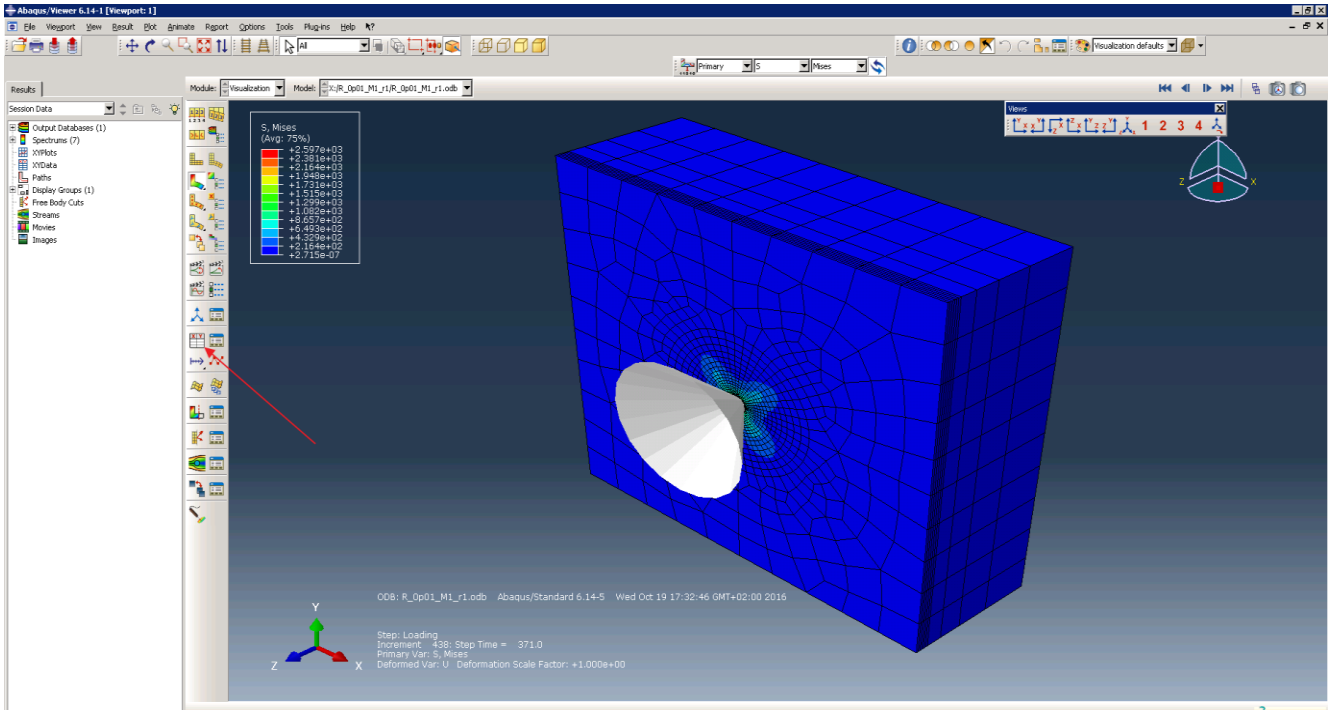
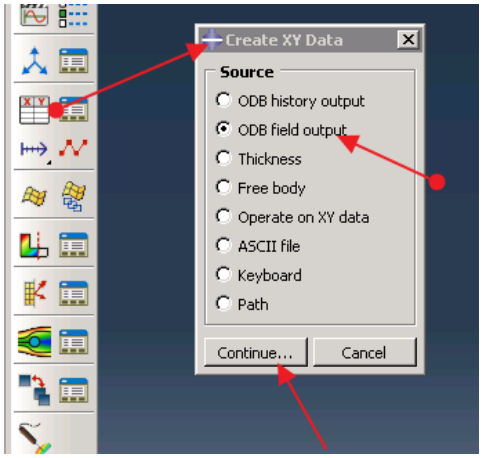
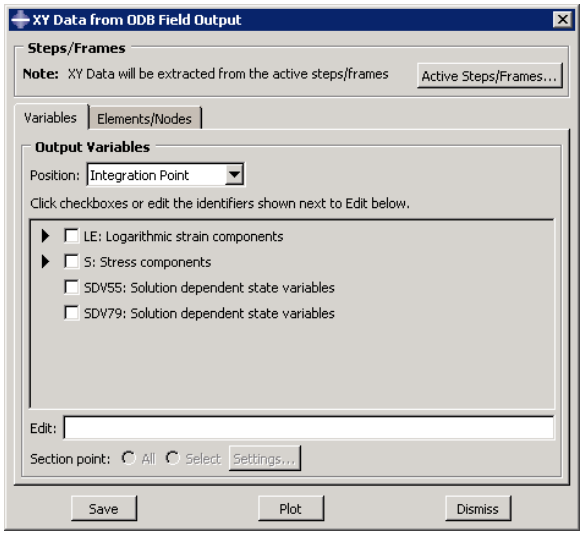


Fig. 3.1 make sure the block in ODB can be deformed, then deal with XY data

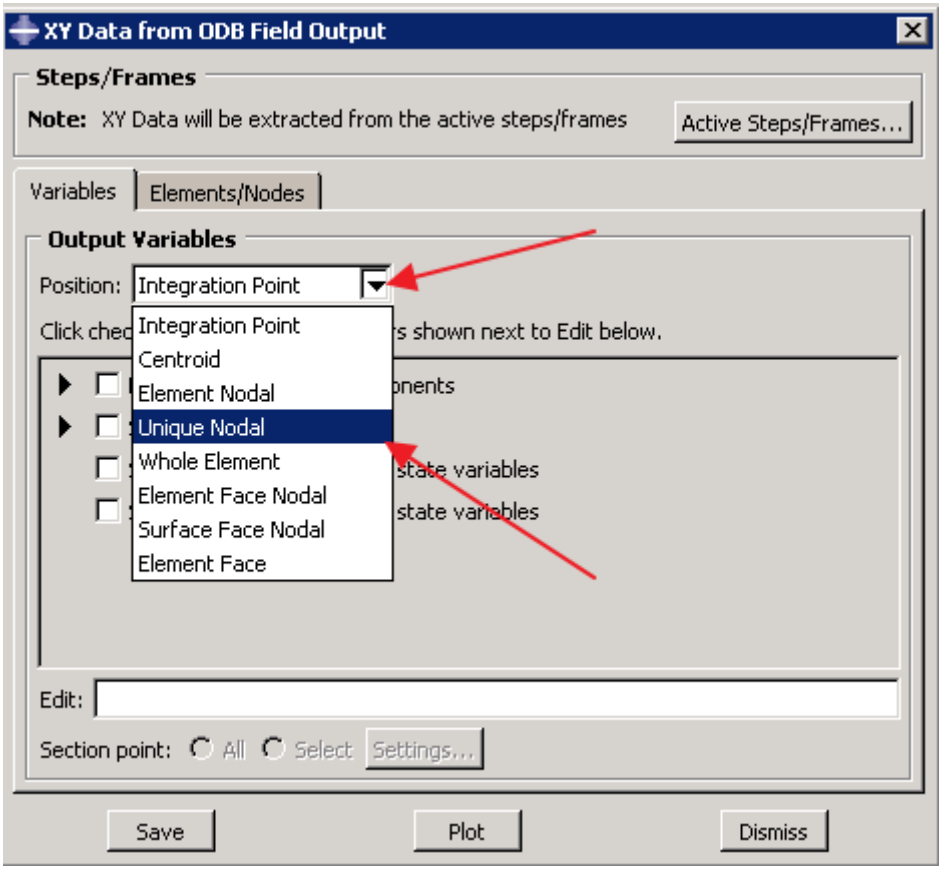
4) Click “continue” under “ODB feld output”



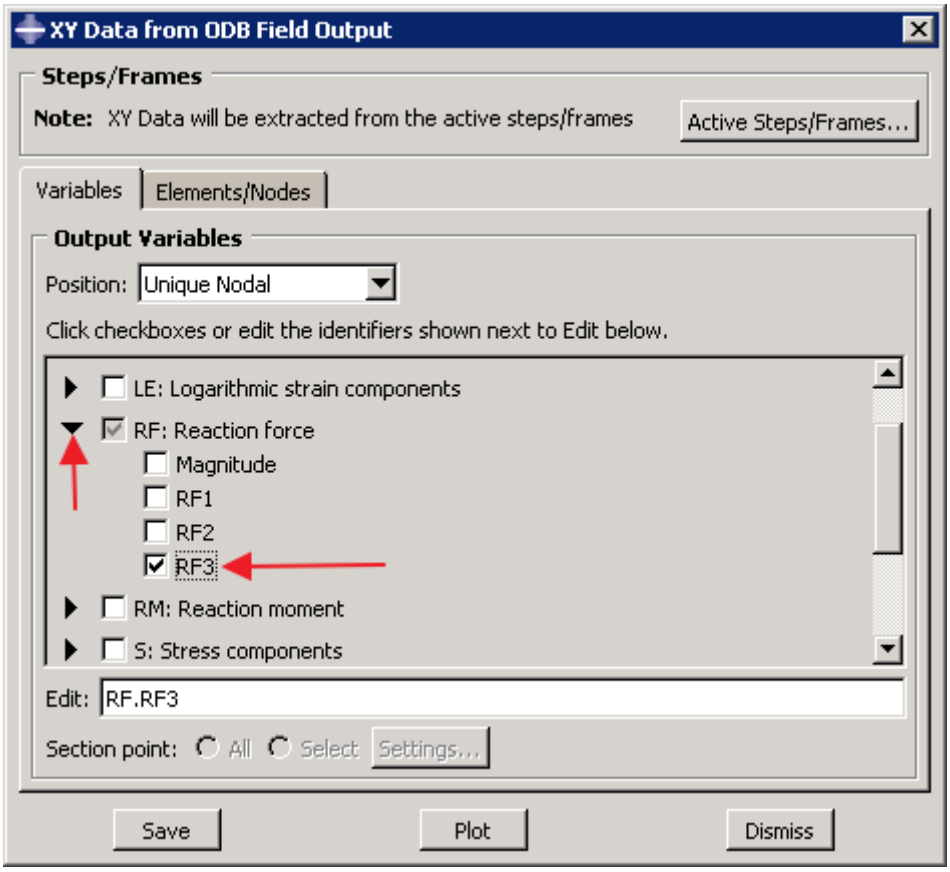
5) Then “XY Data from ODB Feld Output” box appears



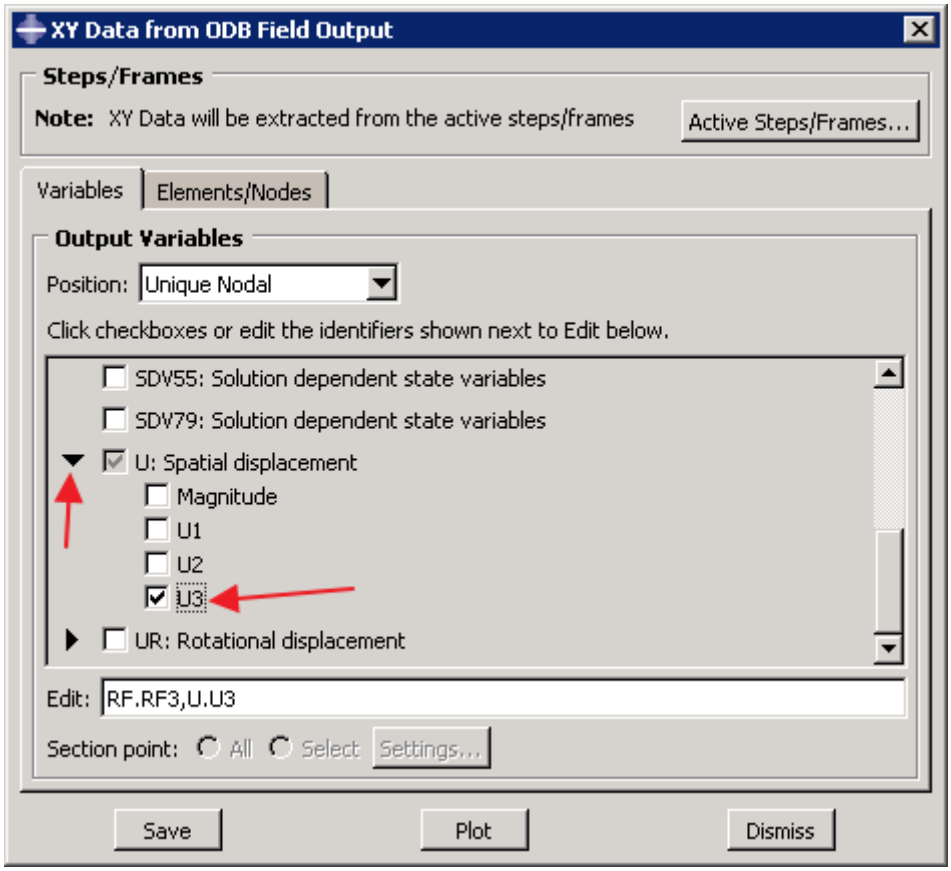
6) Click the black-downwards-arrow, then click “Unique Nodal”. (chose the nodal)



7) Click the black-downwards-arrow, then click “RF”, then click “RF3”. (chose RF3 as the output item, the force in Z direction)



8) Click the black-downwards-arrow, then click “U”, then click “U3”. (chose U3 as the output item, the displacement in Z direction)



9) Click in the sequence in Fig. 3.2. This aims to choose the reference point, then save the data selected in 6), 7) and 8) above.

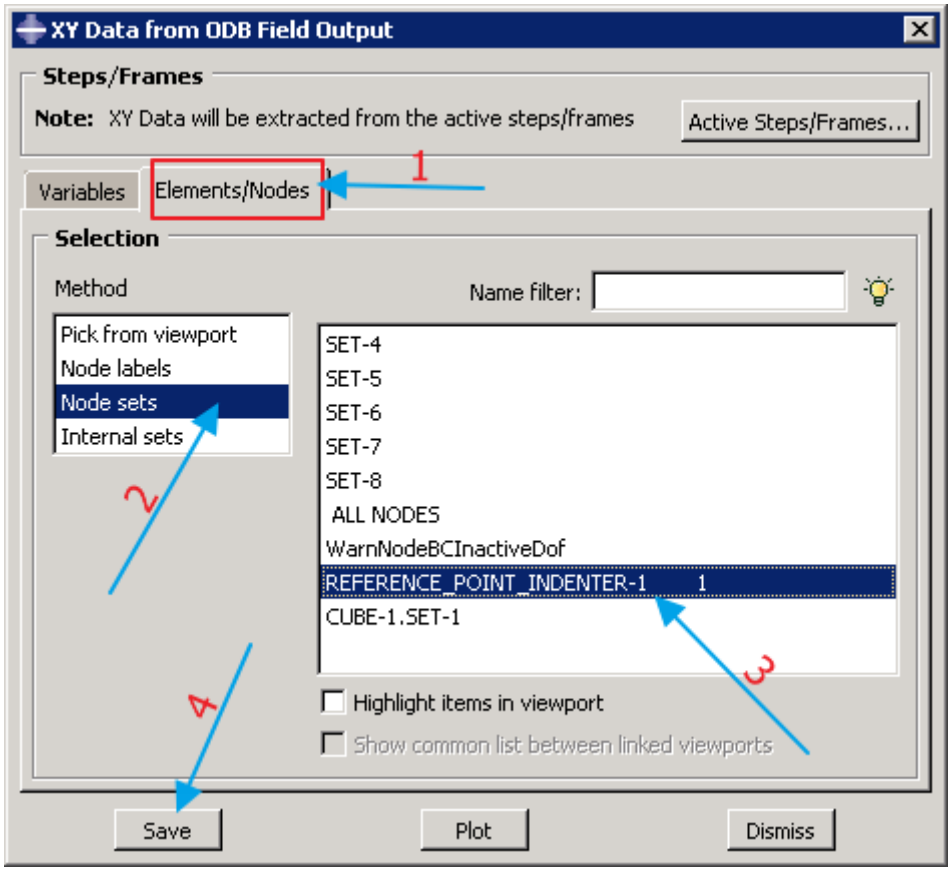
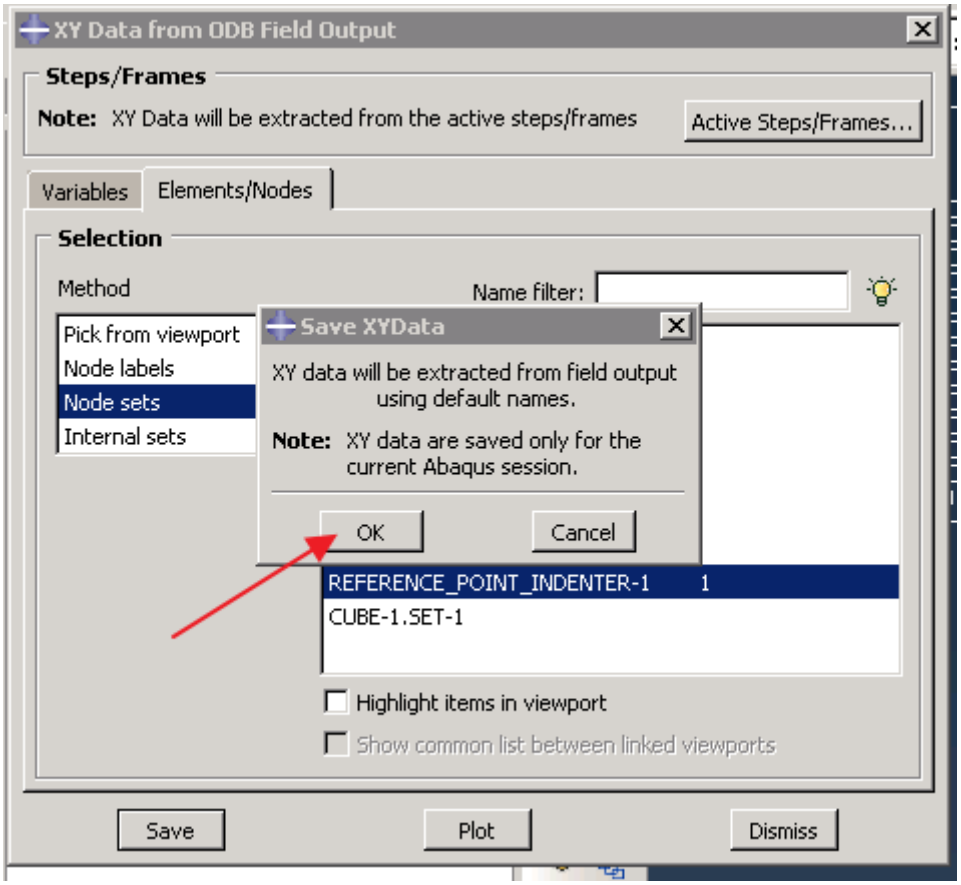
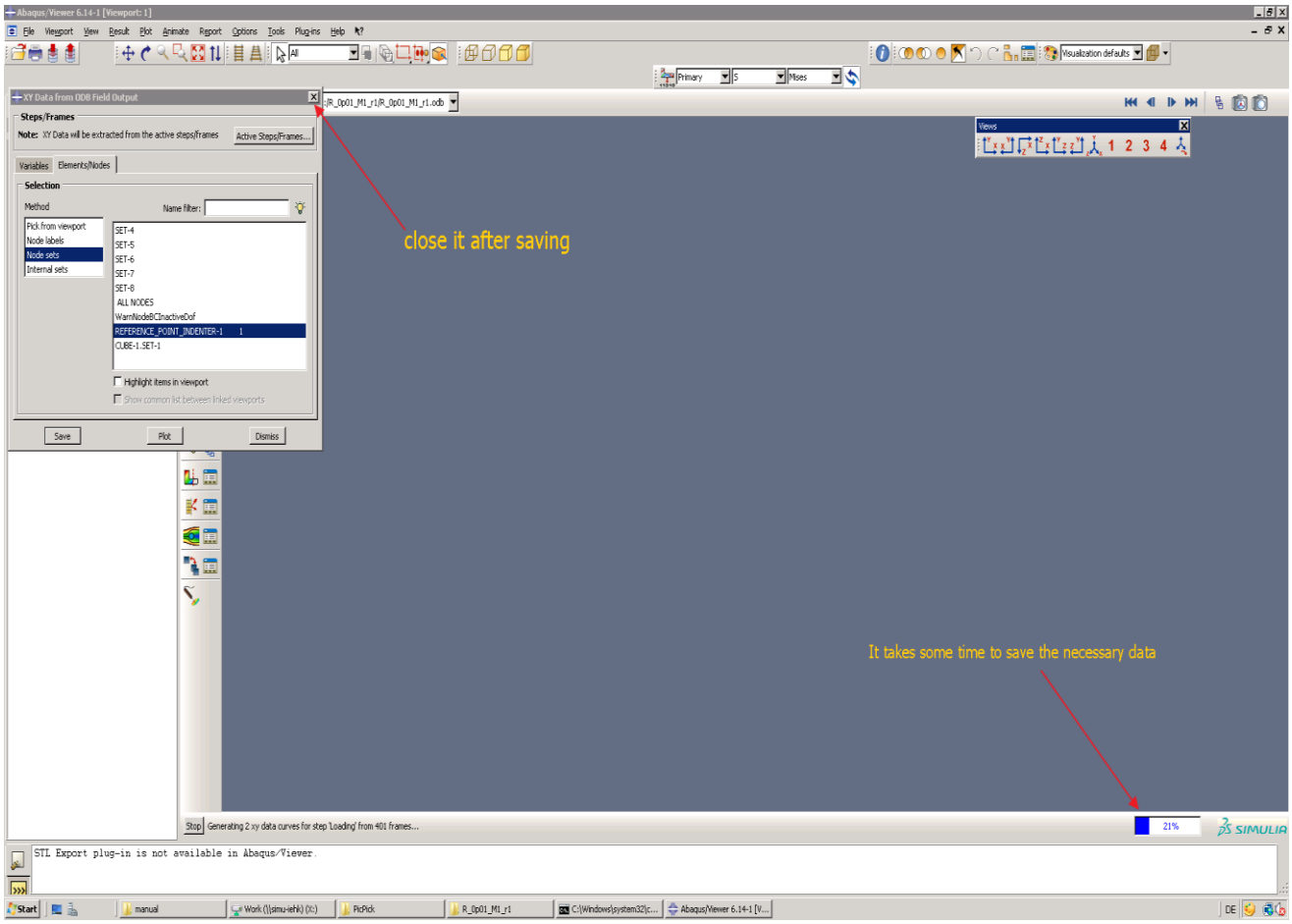


Fig. 3.2 choose the reference point and save

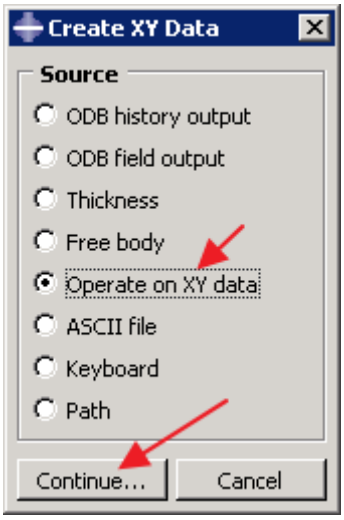
10) Click “OK”



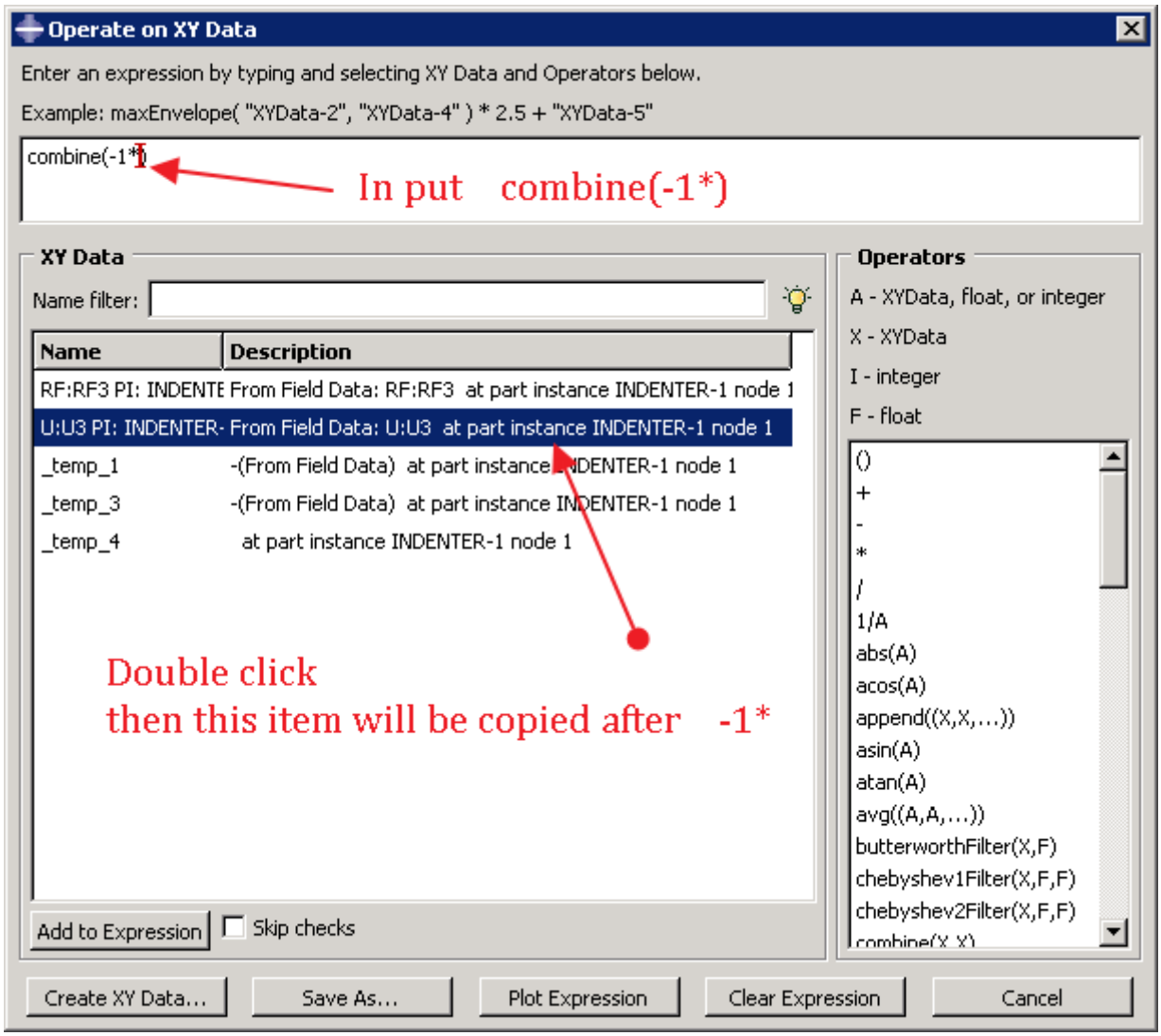
11) It can take several minutes to save the data. You can turn off the “XY Data from ODB Feld Output” box after this.



12) Click “Continue” after toggling on “Operate on XY data” to call up the data for plotting load-displacement curve



13) Type “comobine(-1*)”, then double click U item (the whole item is the marked blue) to copy this item after *. This means set -U3 as X values.



14) Similarly put R3 in the expression in 13) above. This means to set –RF3 (reference force in Z direction) as the Y values. Use Komma "," (no SPACE neither before nor after Komma) to separate U3 and RF3. The whole expression is like that in Fig. 3.3. You can click "Plot Expression" to check whether the load-displacement curve is good enough

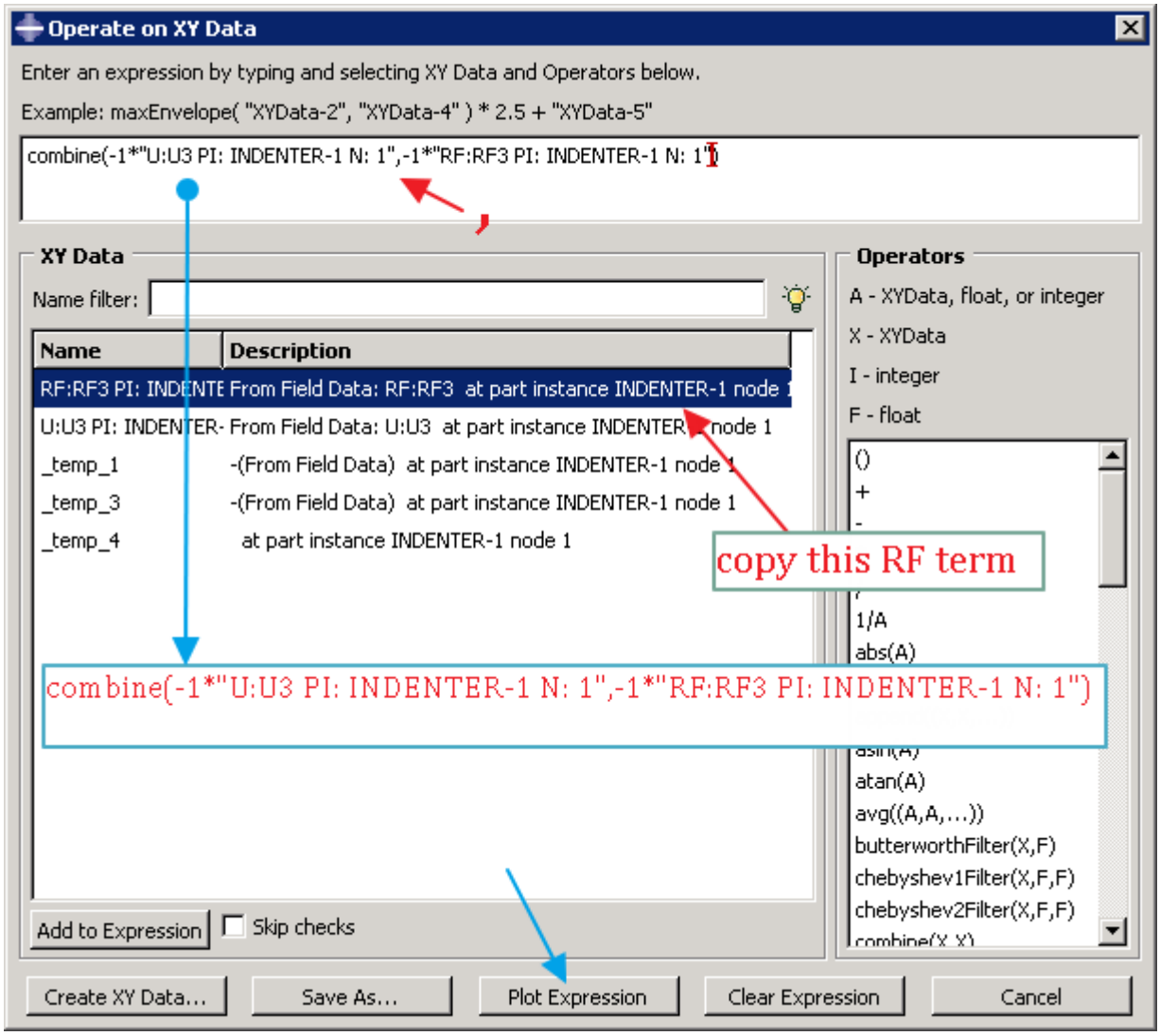
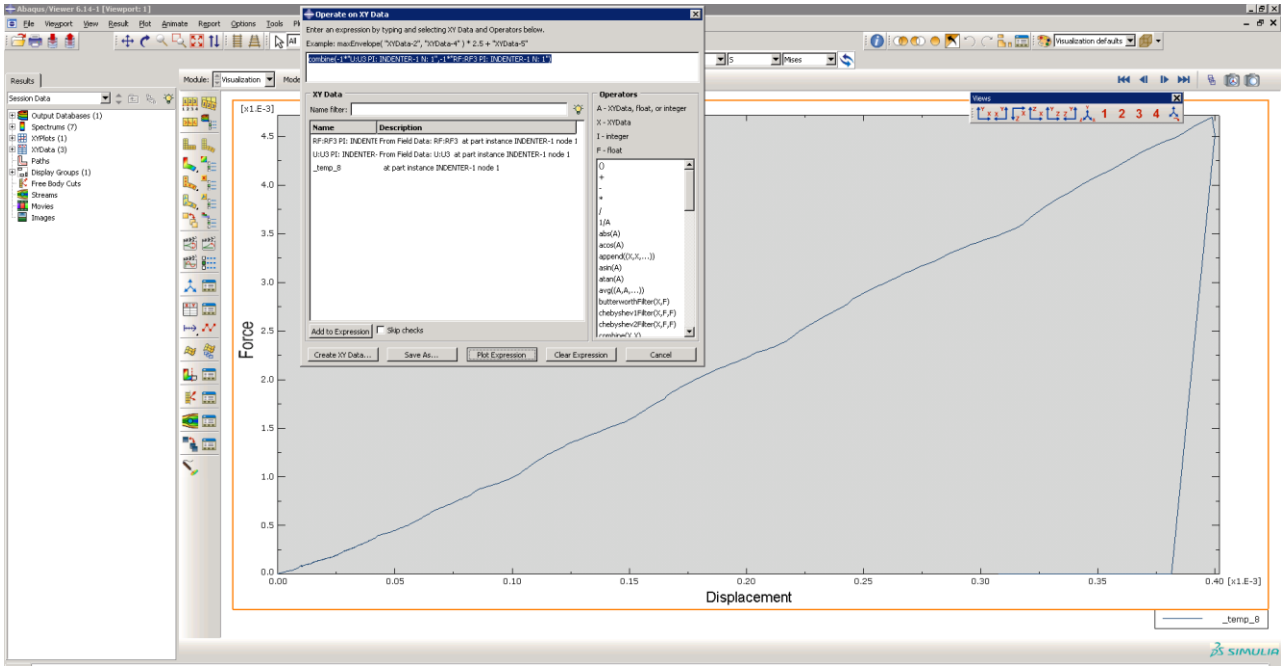


Fig. 3.3 expression

15) The load-displacement curve is then plotted



16) If you are pleased with the result, then save the data with a name you can identify e.g. “Ph_tutor” as shown in Fig. 3.4.

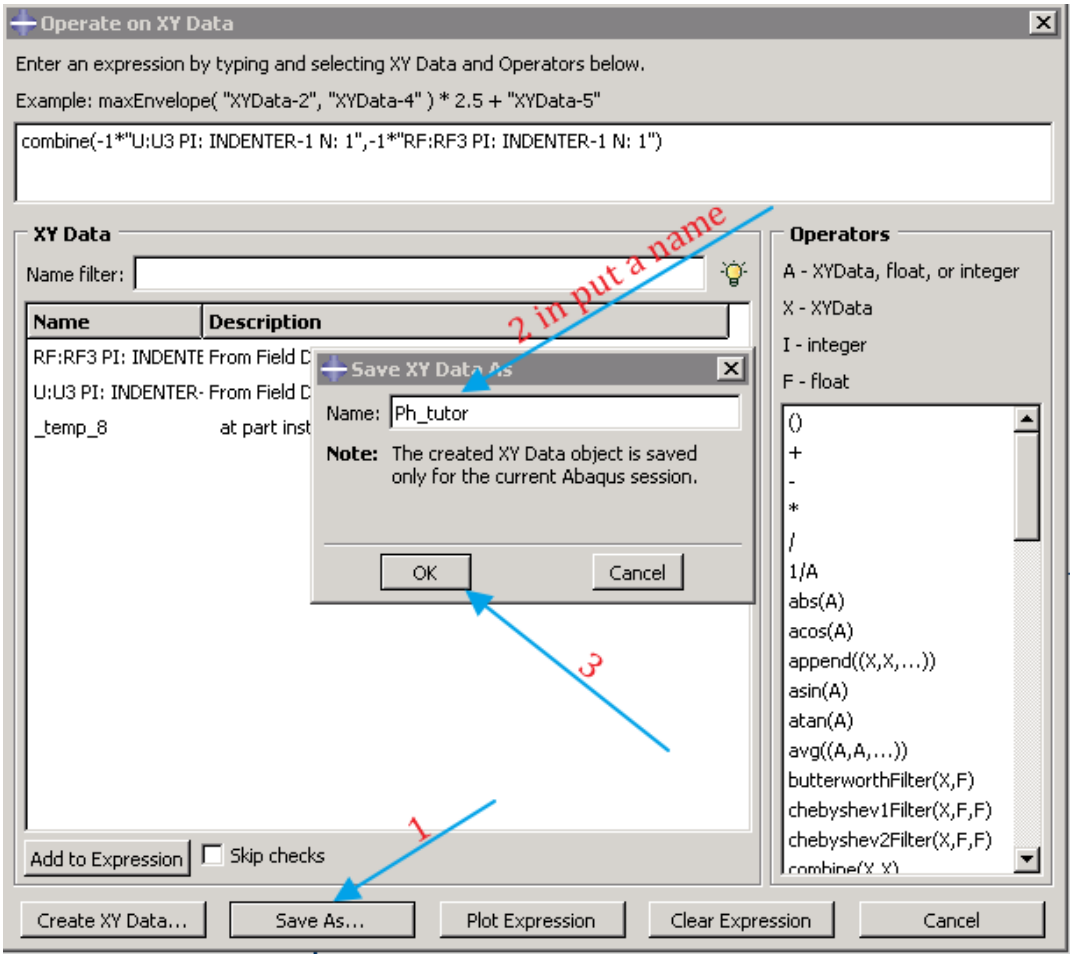
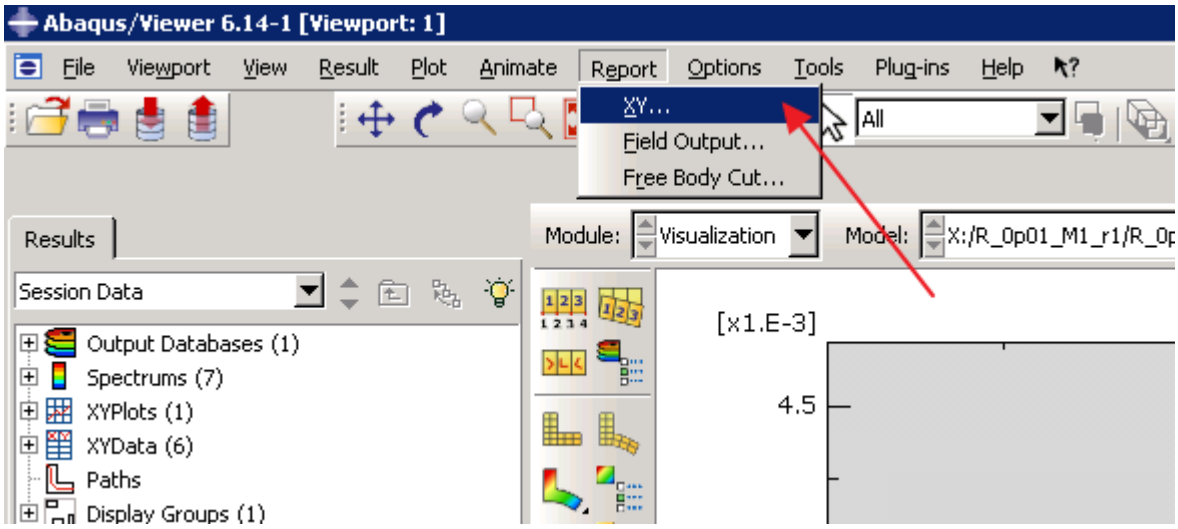
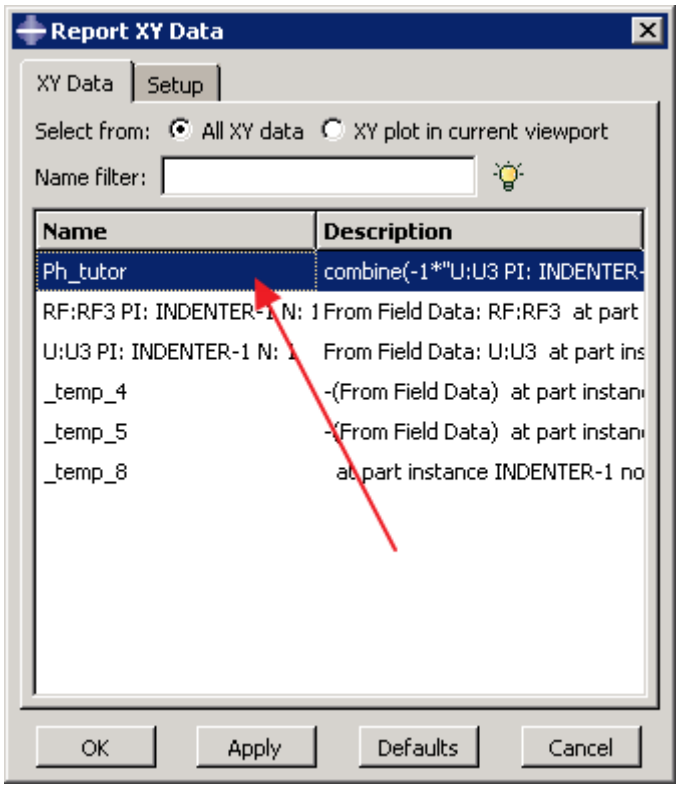


Fig. 3.4 click in this sequence to save the data you are pleased with.

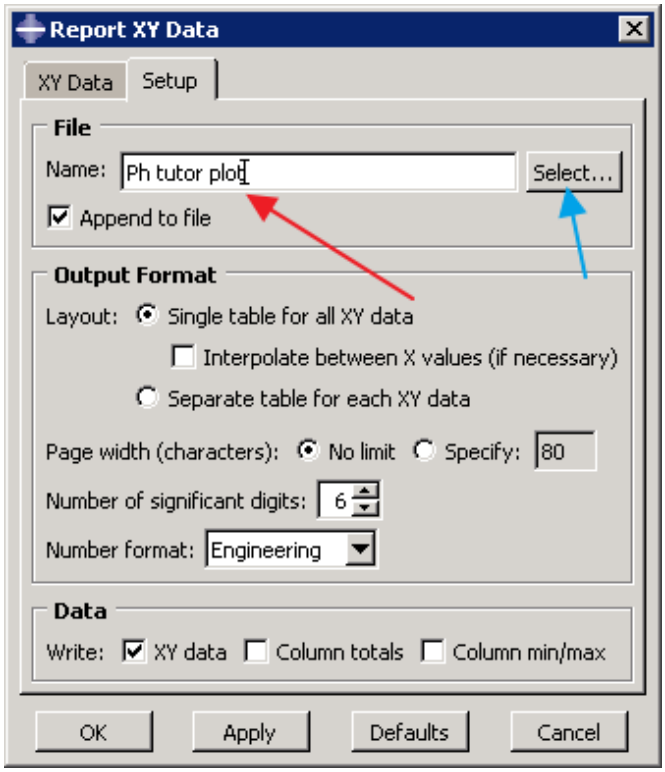
17) Click “XY” to report XY



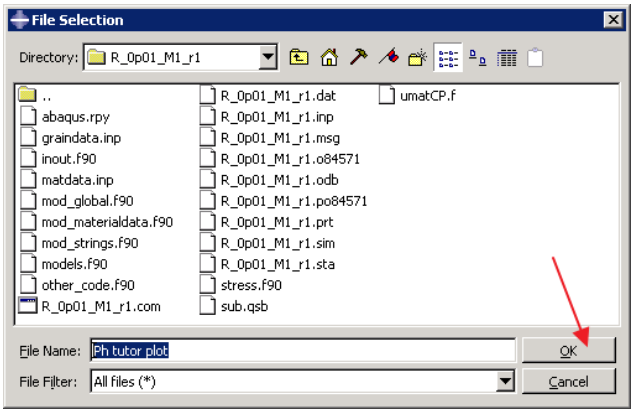
18) “Report XY Data” box appears, click “Ph_tutor” to select this item under “XY Data”.



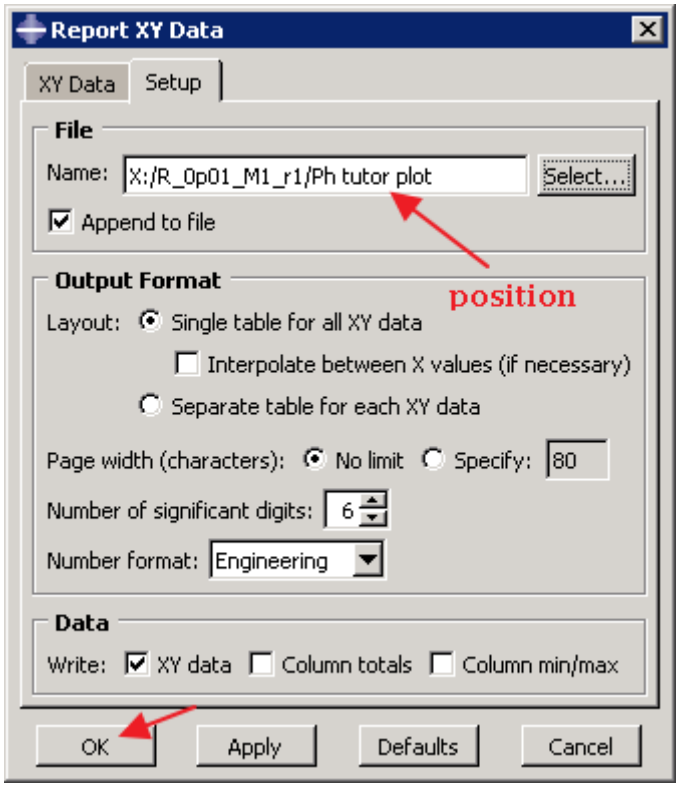
19) Give a name of the save file e.g. “Ph tutor plot”, if you are not sure about the routine i.e. the folder where this file will be saved, click “select” to check or change the rountine.



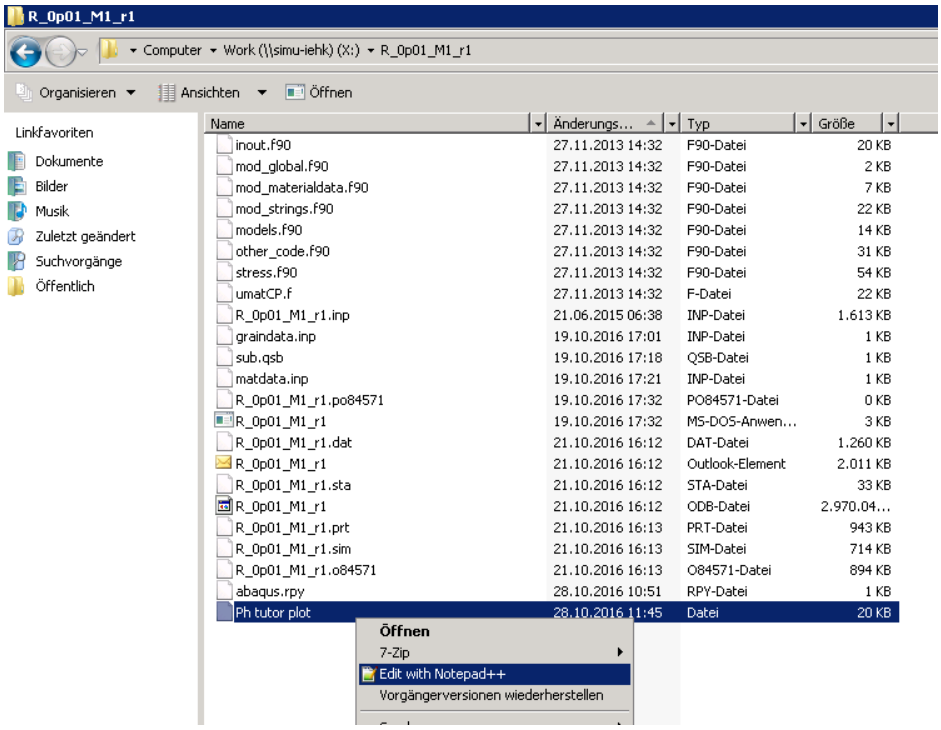
20) If you can find the file in which “Ph tutor plot” will be saved, click “OK”.



21) Click “OK” to save “Ph tutor plot”



22) Open the file in the folder with Notepad.



23) This is the content of “Ph tutor plot”

X:\R_0p01_M1_r1\Ph tutor plot - Notepad++

File Edit Search View Encoding Language Settings Macro Run Plugins Window

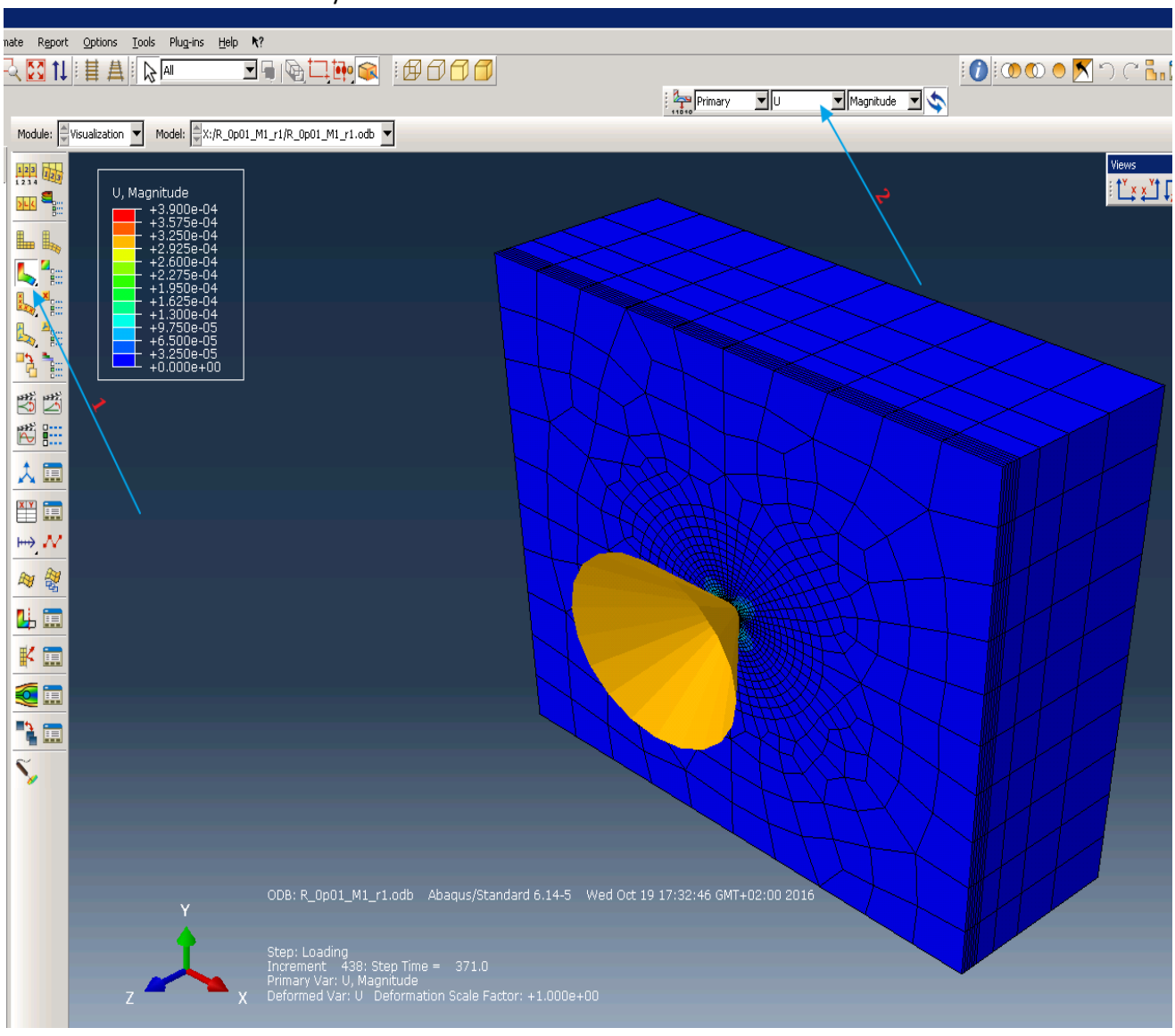
Ph tutor plot

	X	Ph_tutor
1		
2		
3		
4	-0.	0.
5	2.E-06	12.6201E-06
6	4.E-06	29.726E-06
7	6.E-06	39.3776E-06
8	8.E-06	57.1902E-06
9	10.E-06	89.7284E-06
10	10.E-06	81.1768E-06
11	10.E-06	78.6591E-06
12	10.E-06	77.2722E-06
13	10.E-06	76.2783E-06
14	10.E-06	75.5121E-06
15	10.E-06	75.5121E-06
16	10.3917E-06	81.4878E-06
17	10.3917E-06	79.3205E-06
18	10.3917E-06	78.0752E-06
19	10.3917E-06	77.1495E-06
20	10.5703E-06	84.4957E-06
21	10.7785E-06	87.3691E-06
22	10.9868E-06	89.1134E-06
23	11.195E-06	90.7653E-06

4. Plot Pile-Ups

Complete the following steps to select, extract and plot pile-up

1) Present the deformed assembly under “U” mode



2) Click in the sequence in Fig. 4.1 to present the cube.

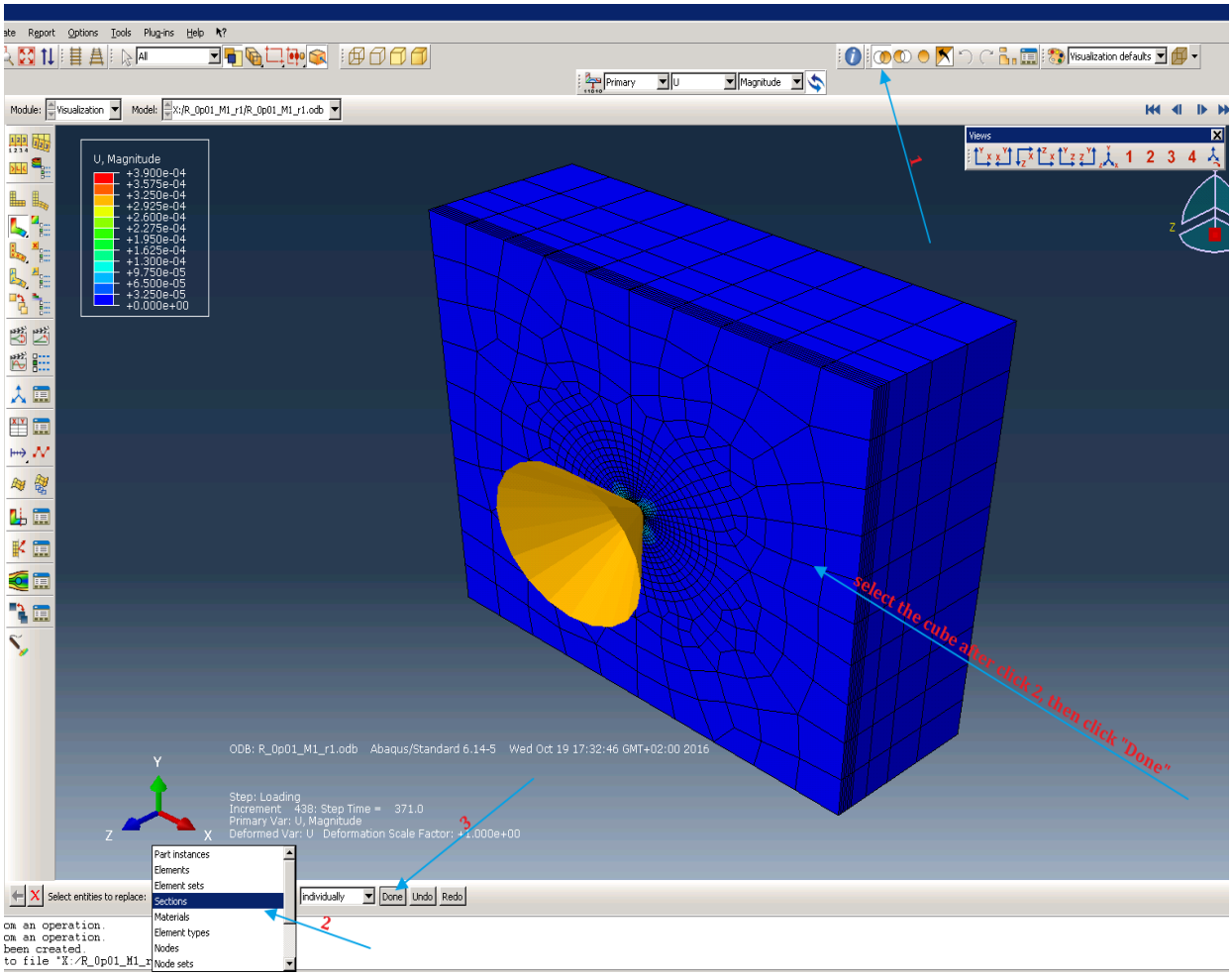
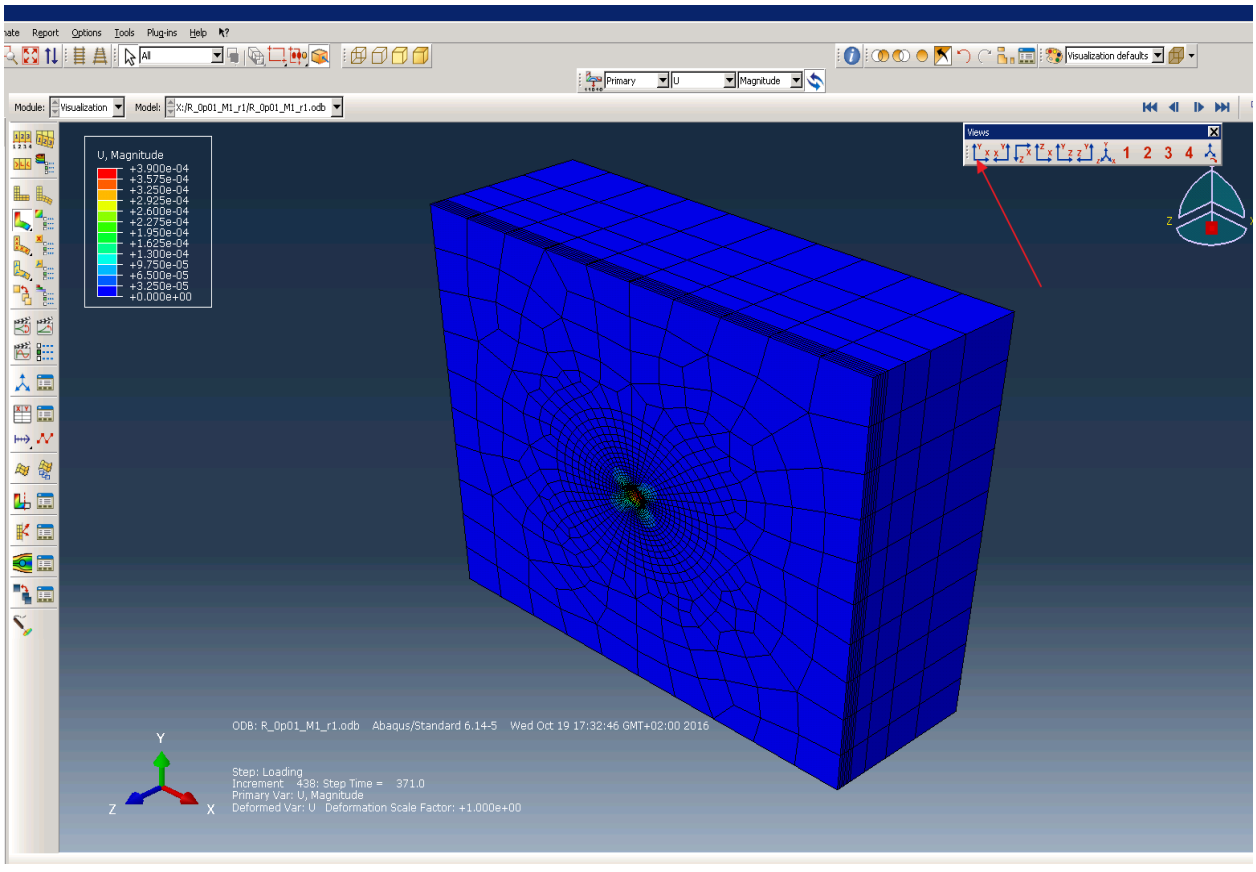
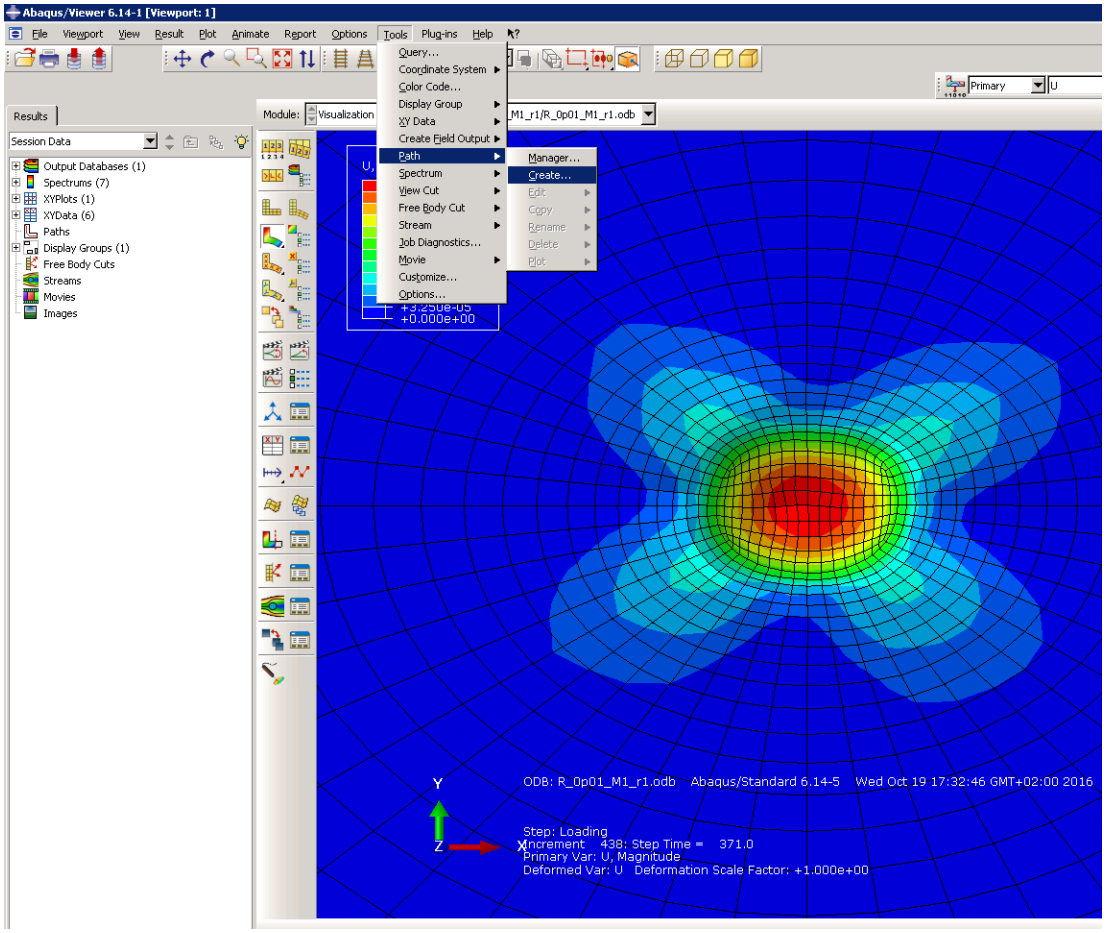


Fig. 4.1 attention: after click 2, click the tube (to select the cube), then perform click 3

3) The deformed cube is then presented. You can click xy view means and magnify to have a better view of the deformed zone.



4) Create a path



5) Do as in Fig. 4.2. Give a name you know e.g. “Pile up tutor”.

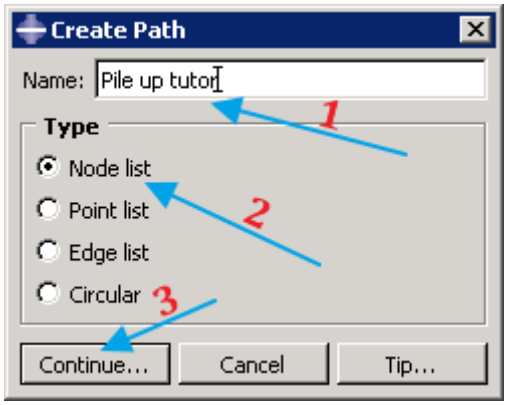
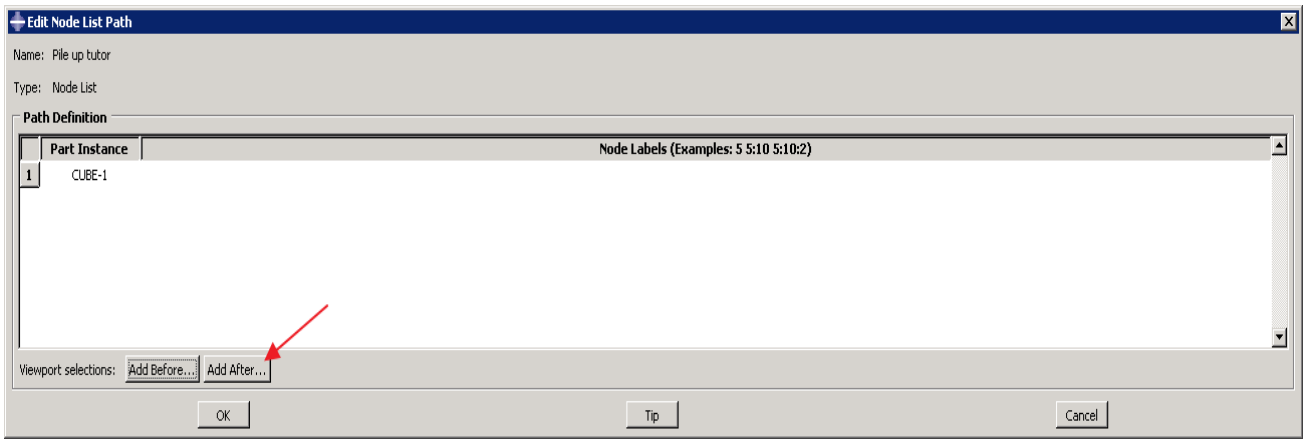


Fig. 4.2 give a name of the path, select node list, then continue

6) Click “Add After” under ”Edit Node Liad Path” box



7) Click the nodes one by one in one direction. These nodes will be saved in the path you have named in 6) above. ABAQUS generates the red line between the adjacent nodes you have clicked. As a result a red line in Fig. 4.3 is the path you would like to create. Click “done” when you think this path is good enough.

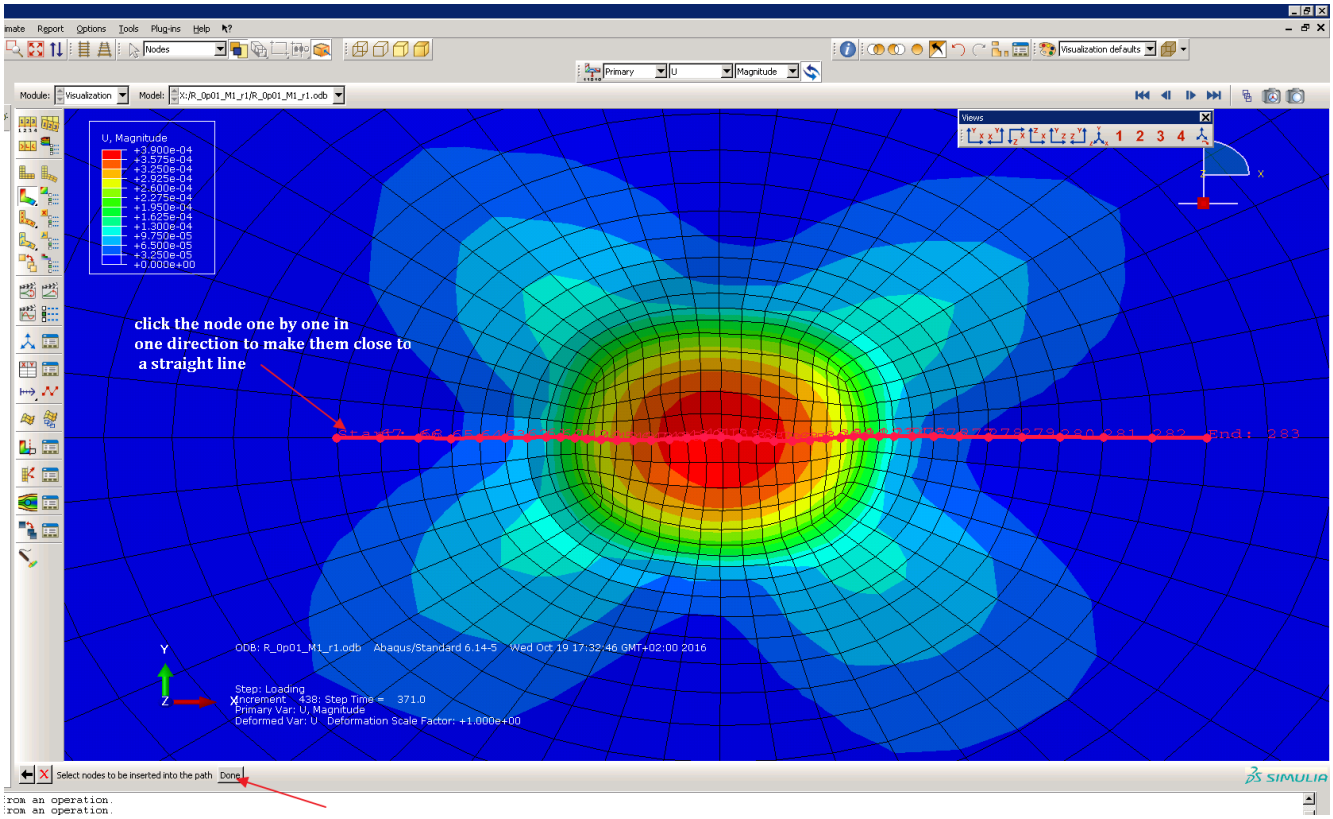
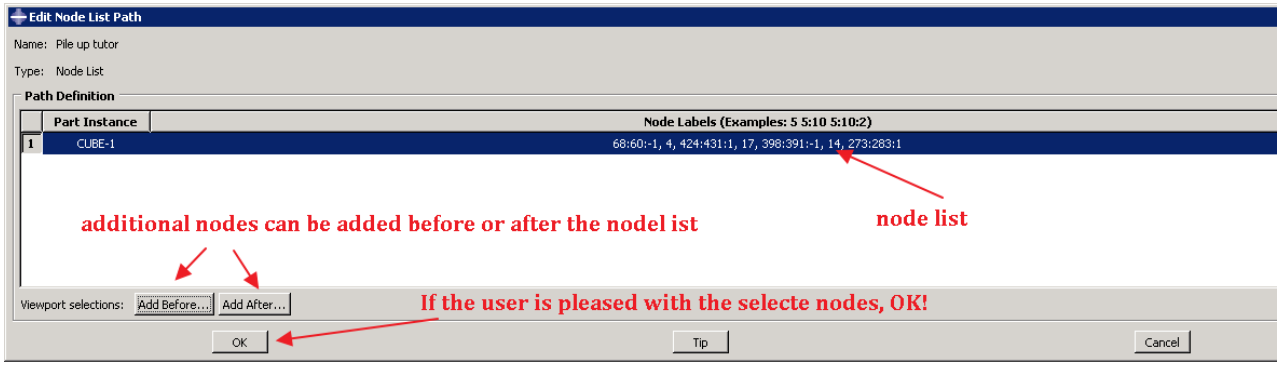
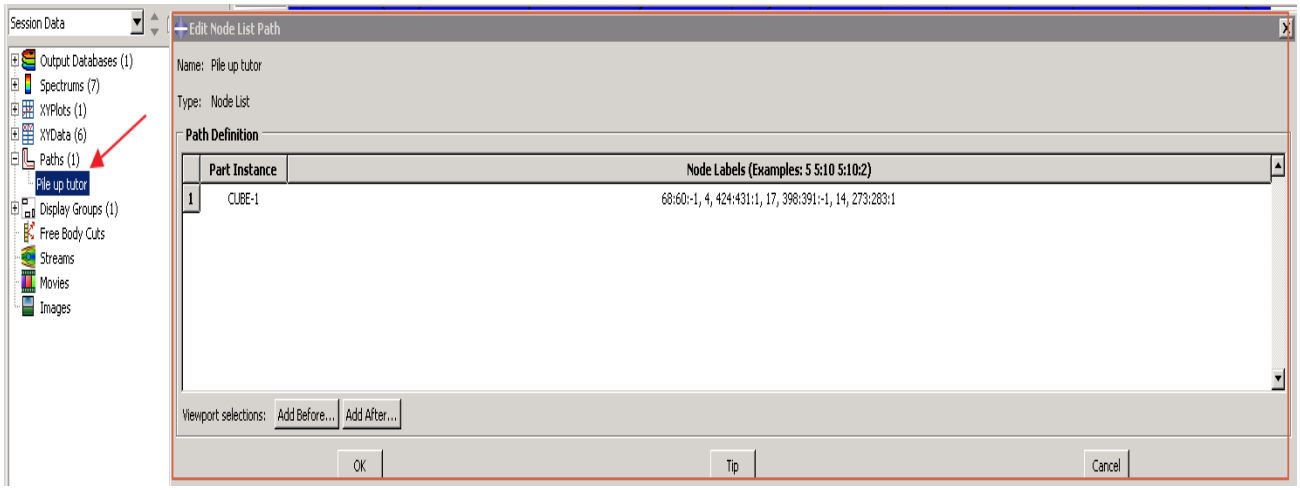


Fig. 4.3 click the nodes to create the path

8) This path could be further edited by adding additional nodes before or after this node list. Click “OK” after the edition to save the path.



9) Further edition could be done after saving



10) Click as in Fig. 4.4 to deal with the path

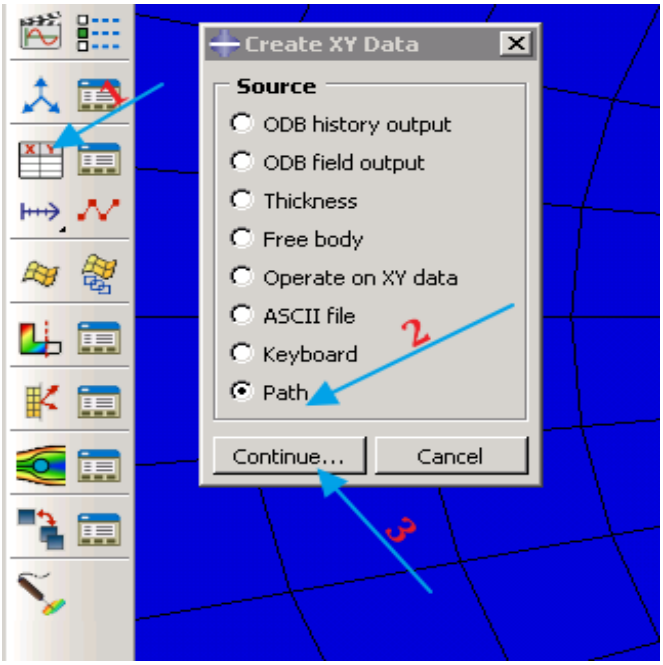
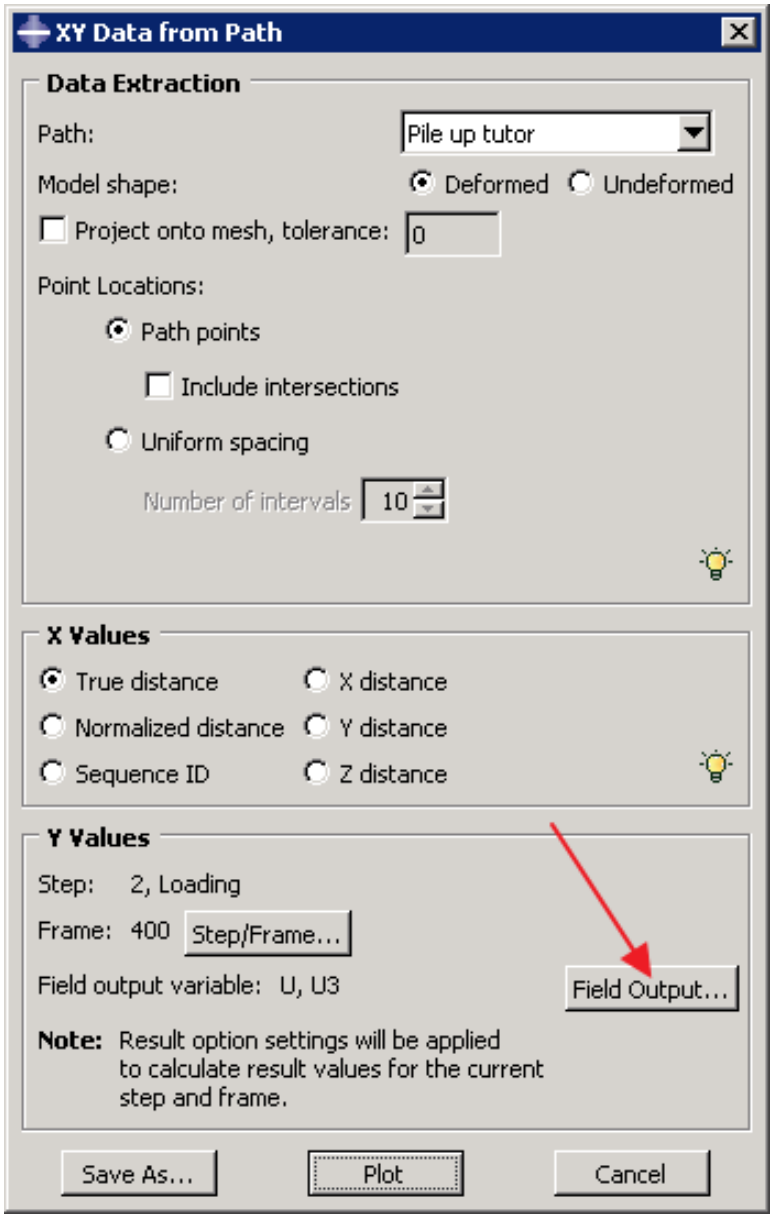


Fig. 4.4 click in sequence

11) Click “Feld Output” under “XY Data from Path”



12) Click in sequence as in Fig.

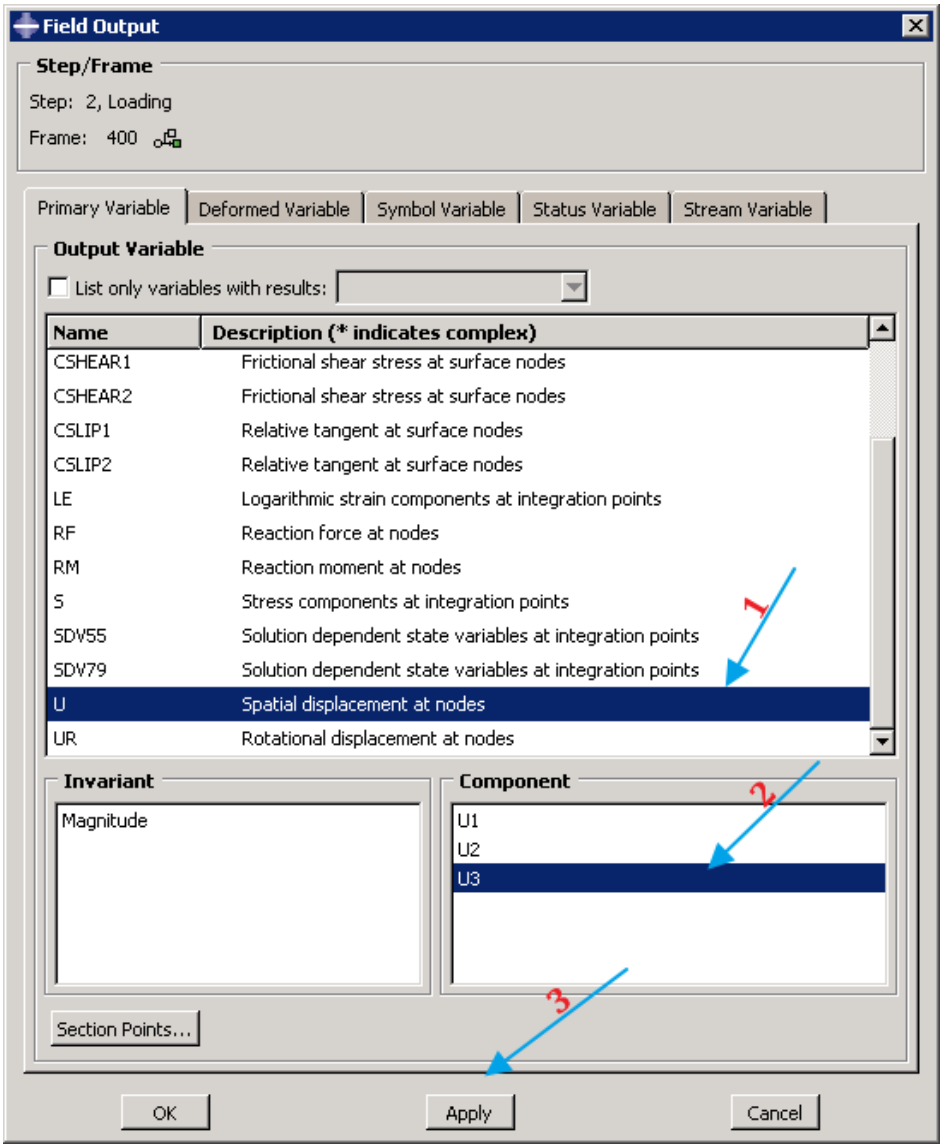
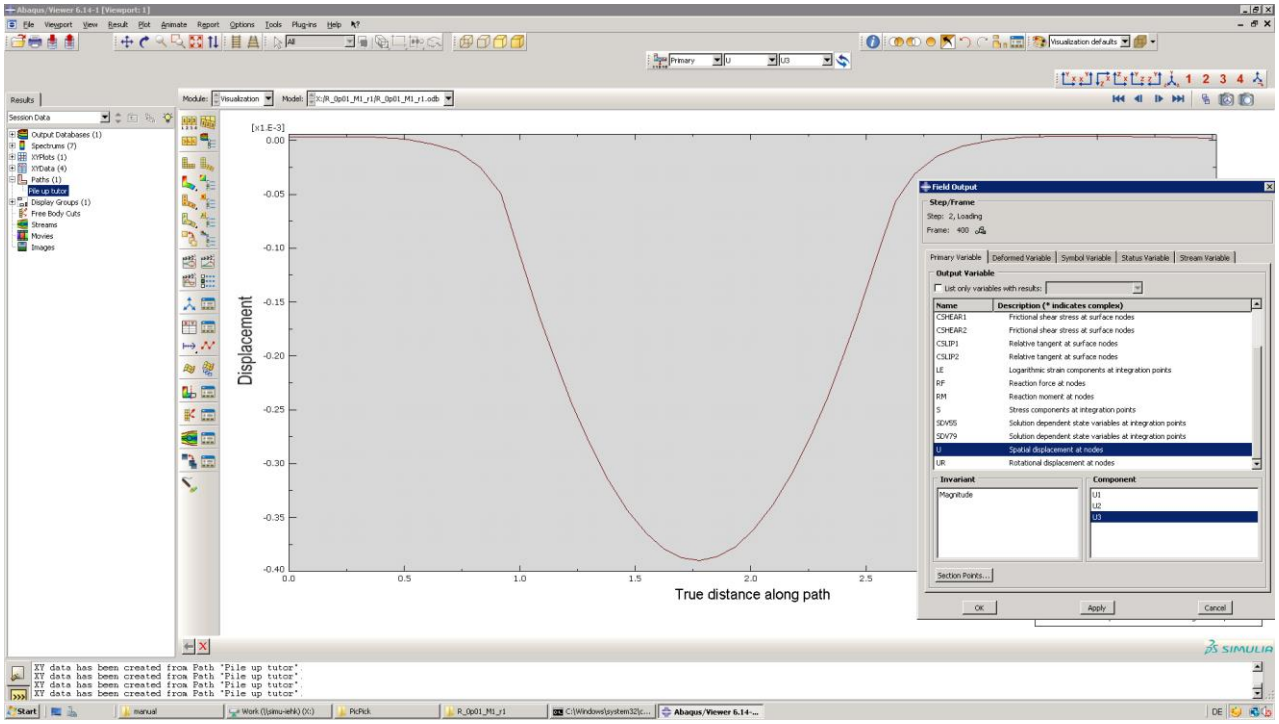
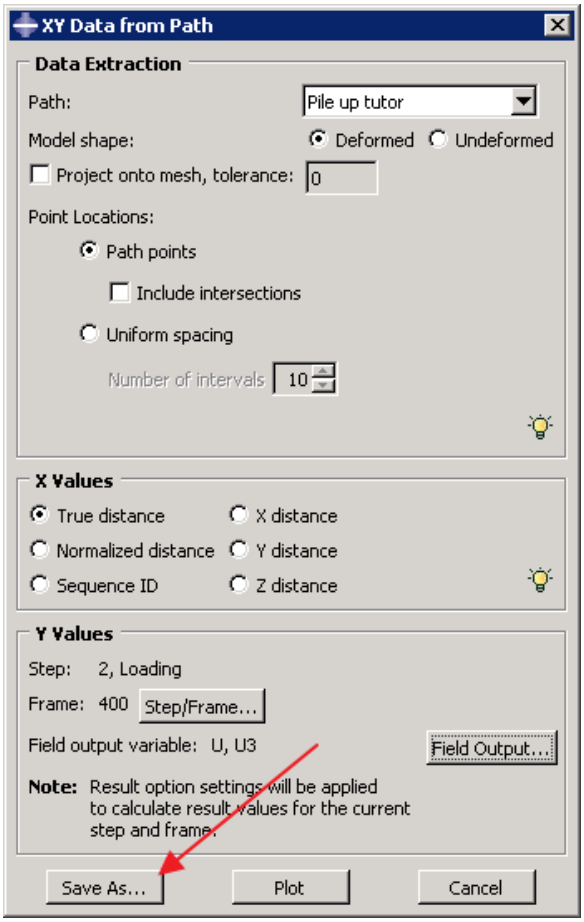


Fig. 4.5 click in sequence to select U3

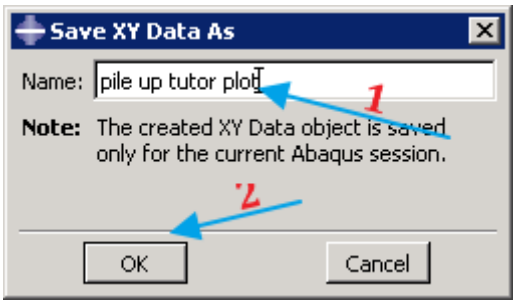
13) The pile-up ris then plotted



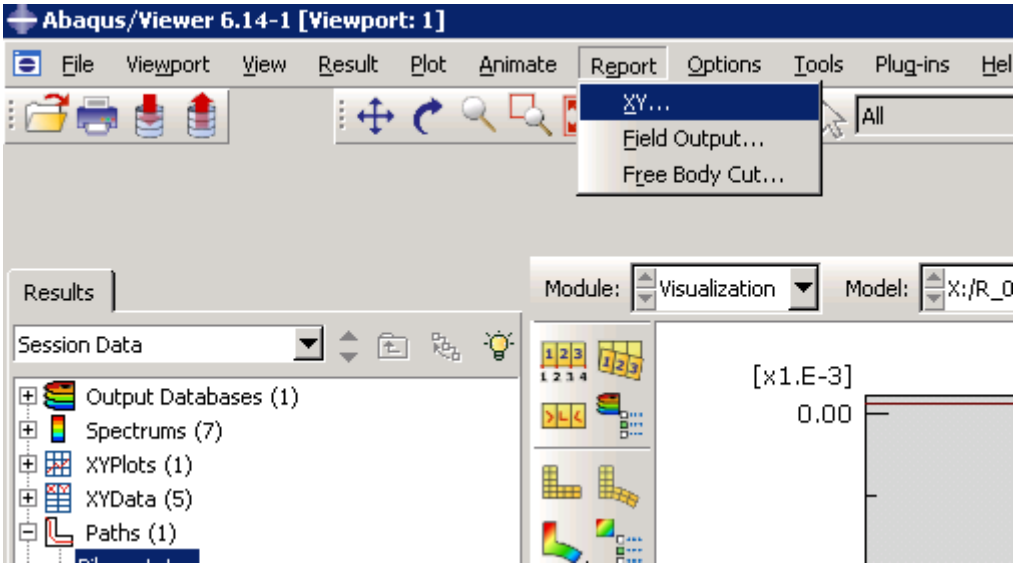
14) If you are pleased with the pile-up in the path you've selected, you can save this data by clicking "Save As"



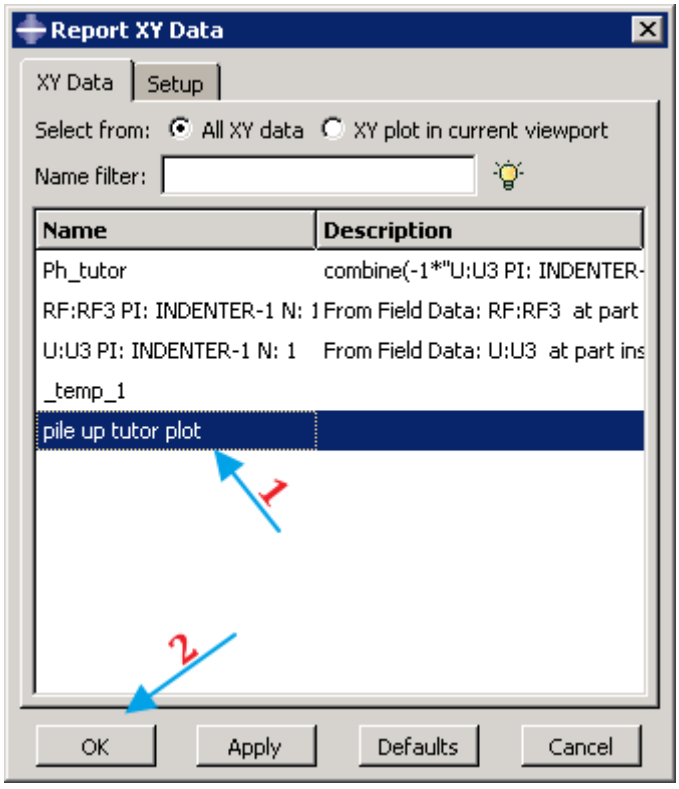
15) Give a name you can identify e.g. "pile up tutor plot", then click "OK".



16) Click "Report XY" to report the pile up data



17) Select “pile up tutor plot” as the one you’d like to report, click “OK”.



18) Click as in sequence as in Fig. 4.6

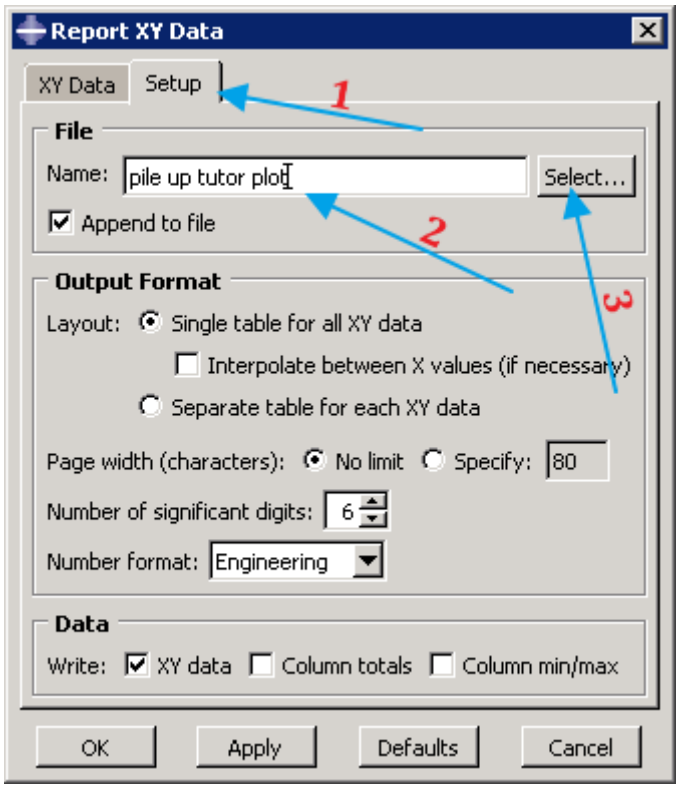
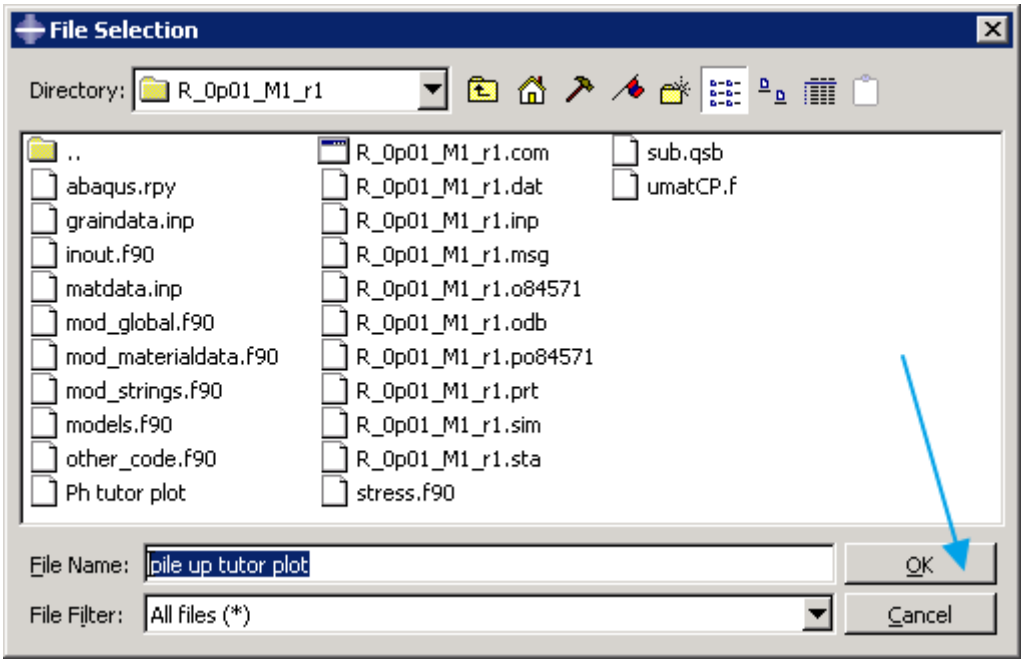
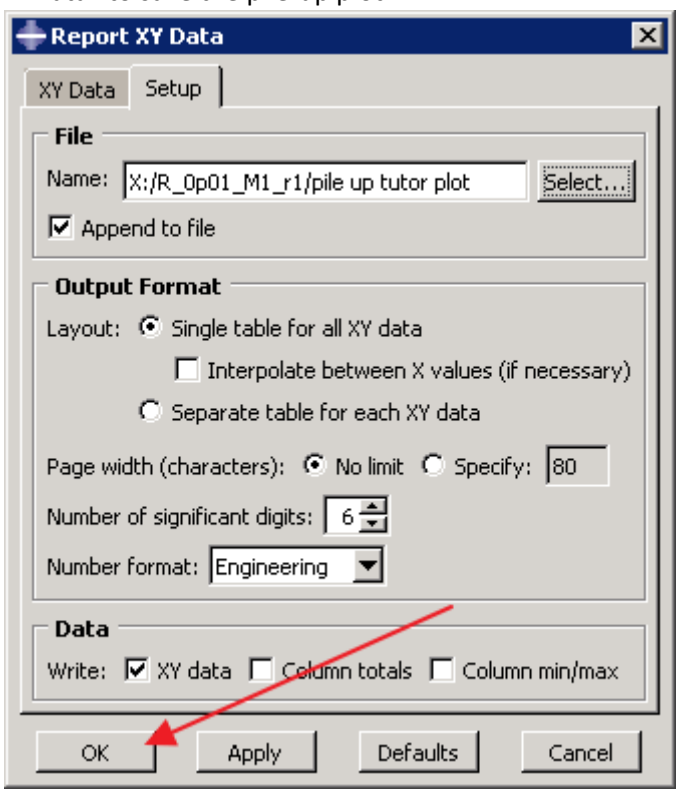


Fig. 4.6 click 3 is for checking the routine i.e. the file where this data is to be saved

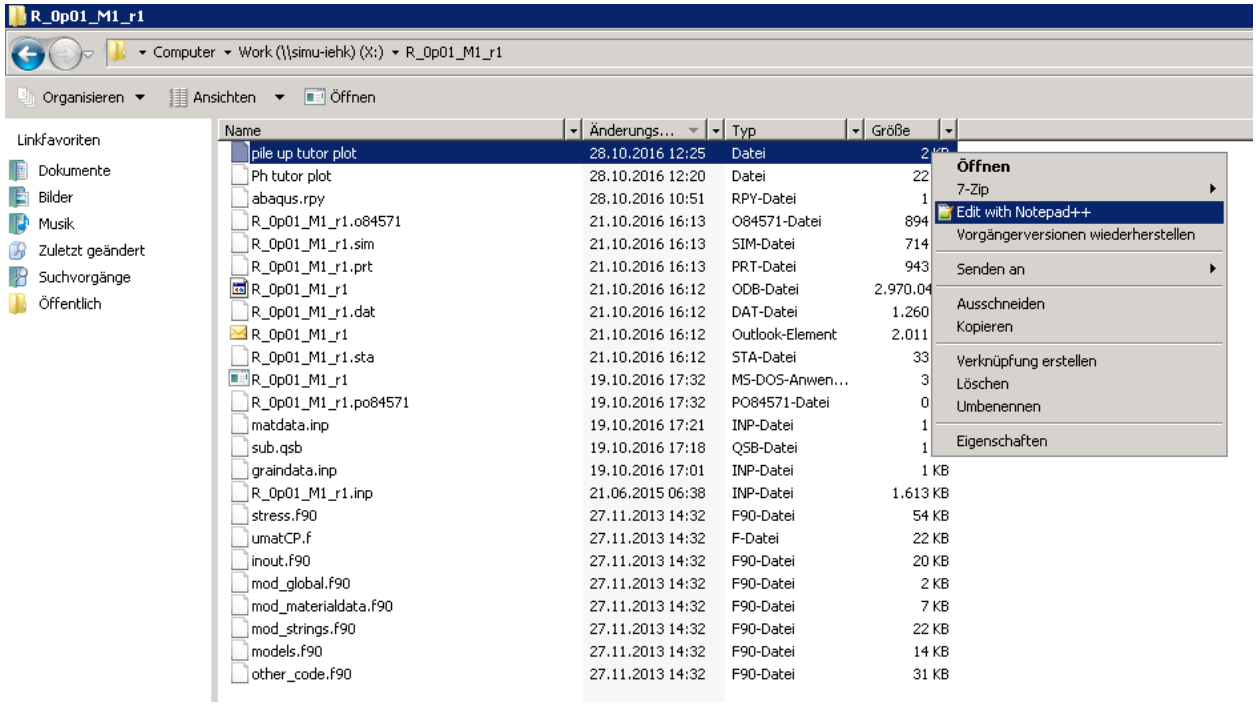
19) If you are sure you can find the data in the file, click “OK” to exit.



20) Click “OK” under “Report XY Data” to save the pile-up plot.



21) Open the file in the folder with Notepad



22) This is the pile-up plot you saved.