Tutorials on DAMASK
Crystal Plasticity Software

Based on lecture notes of Philip Eisenlohr (MSU)

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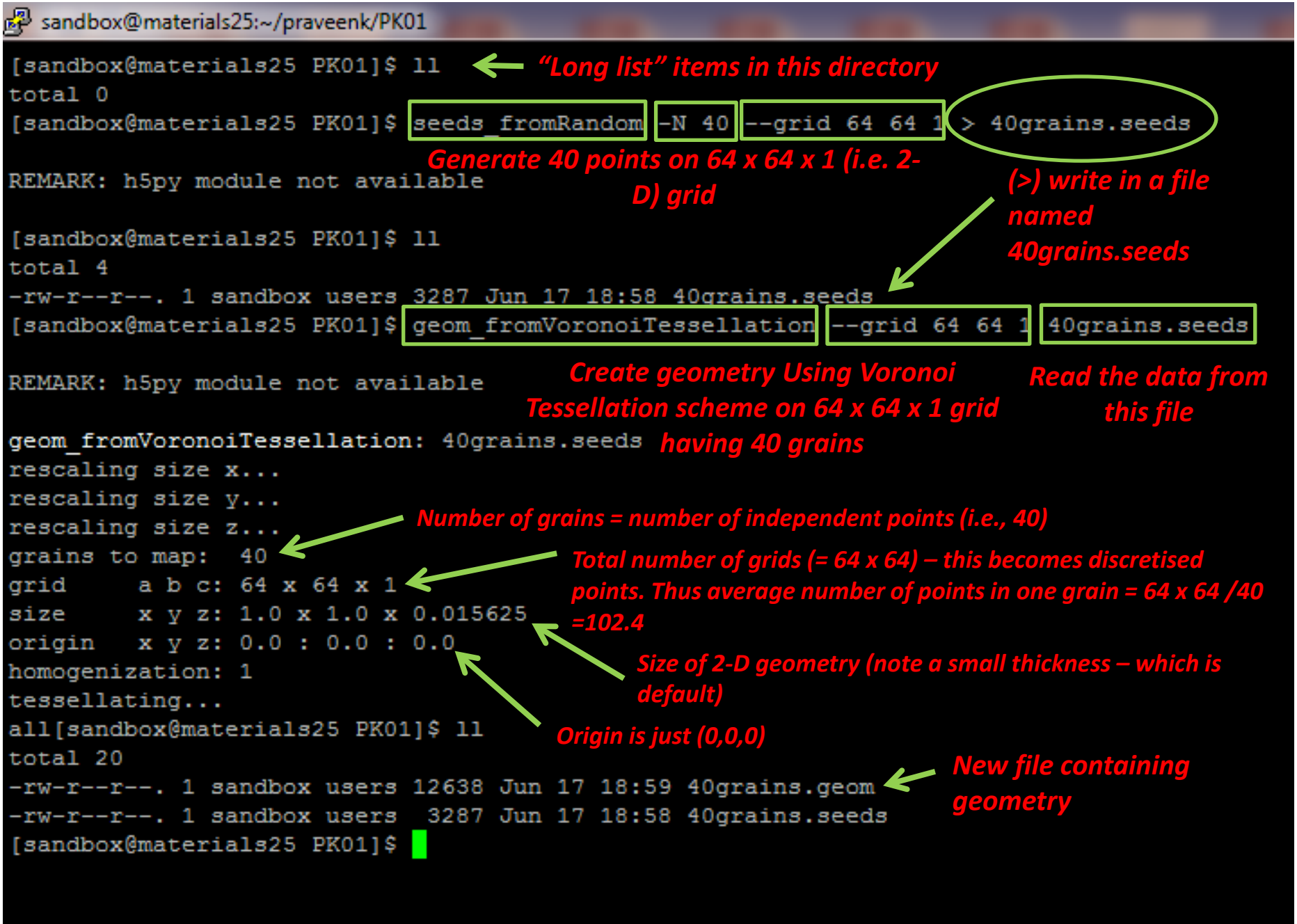
Tutorial 1: Uniaxial tension type loading on an isotropic material (no specific slip system)
Tutorial 2: Uniaxial tension type loading on a crystalline material (specific slip systems, etc.)
Tutorial 3: Uniaxial compression type loading on a 2-phase alloy

Tutorial 1: Uniaxial tension type loading on an isotropic material (no specific slip system)



```
[sandbox@materials25 PK01]$ seeds_check 40grains.seeds

REMARK: h5py module not available

seeds_check: 40grains.seeds
grain data not matching grain count (1)...
rescaling size x...
rescaling size y...
rescaling size z...
[sandbox@materials25 PK01]$ ll
total 24
-rw-r--r--. 1 sandbox users 12638 Jun 17 18:59 40grains.geom
-rw-r--r--. 1 sandbox users  3287 Jun 17 18:58 40grains.seeds
-rw-r--r--. 1 sandbox users  1751 Jun 17 19:29 seeds_40grains.vtu
[sandbox@materials25 PK01]$ geom_check 40grains.geom

REMARK: h5py module not available

geom_check: 40grains.geom
grid     a b c:  64 x 64 x 1
size     x y z:  1.0 x 1.0 x 0.015625
origin   x y z:  0.0 : 0.0 : 0.0
homogenization:  1
microstructures: 40
[sandbox@materials25 PK01]$ ll
total 28
-rw-r--r--. 1 sandbox users 12638 Jun 17 18:59 40grains.geom
-rw-r--r--. 1 sandbox users  3287 Jun 17 18:58 40grains.seeds
-rw-r--r--. 1 sandbox users  2311 Jun 17 19:30 mesh_40grains.vtr
-rw-r--r--. 1 sandbox users  1751 Jun 17 19:29 seeds_40grains.vtu
[sandbox@materials25 PK01]$
```

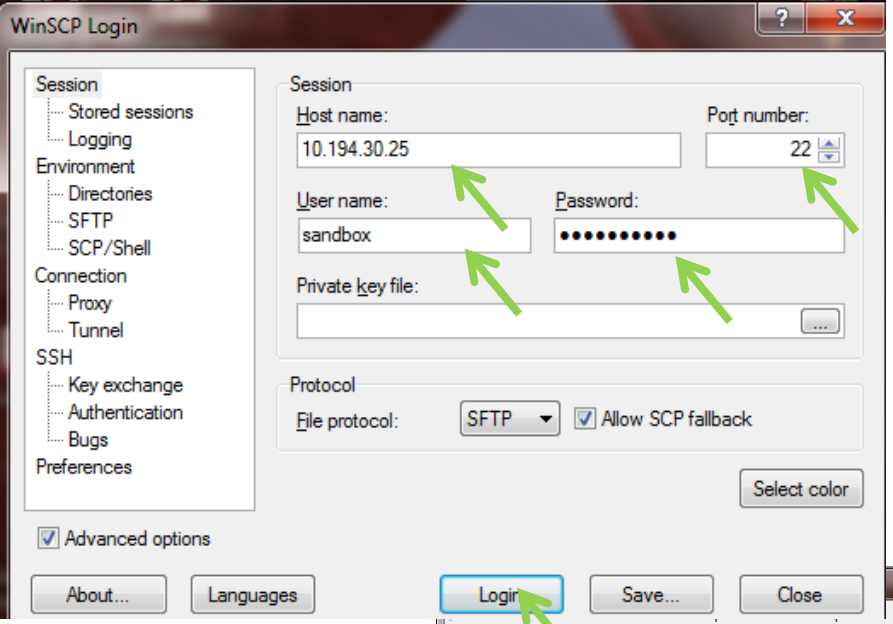
Generates a file (.vtu) which can be opened using "Paraview" to visualize the locations of 40 points

Do not worry about it!

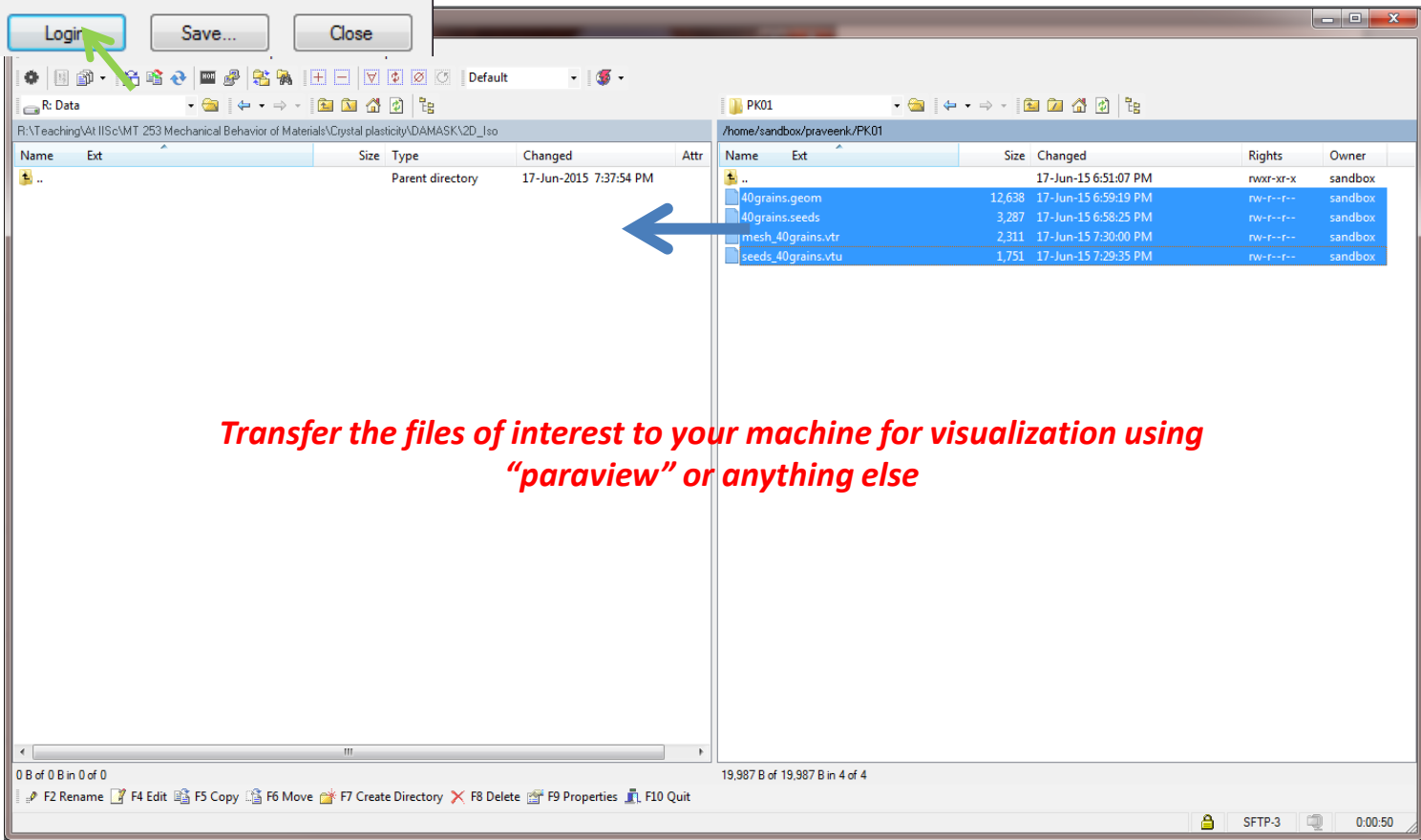
Generates a file (.vtr) which can be opened using Paraview to visualize the 40 grains and how are they formed

No homogenization as each grid lies within a grain

A grain is a microstructure here



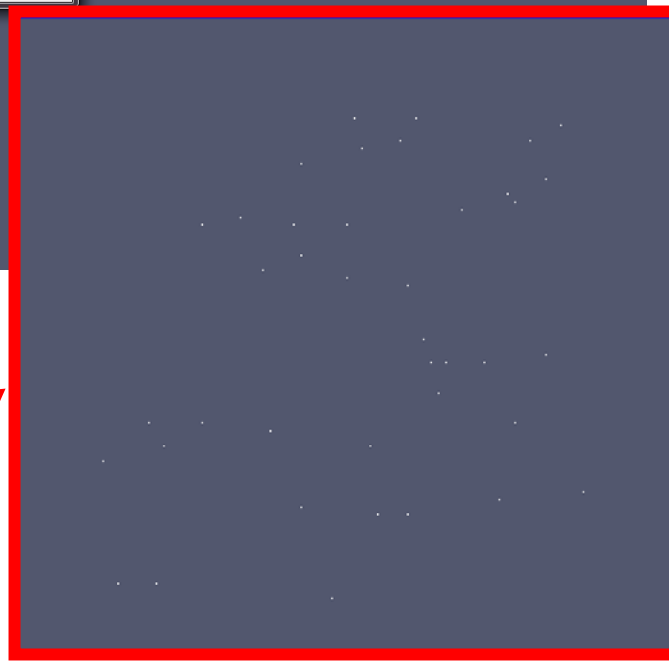
Using SCP program (such as WinSCP) connect to the computer running the program (i.e., 10.194.30.25) using the same login credentials



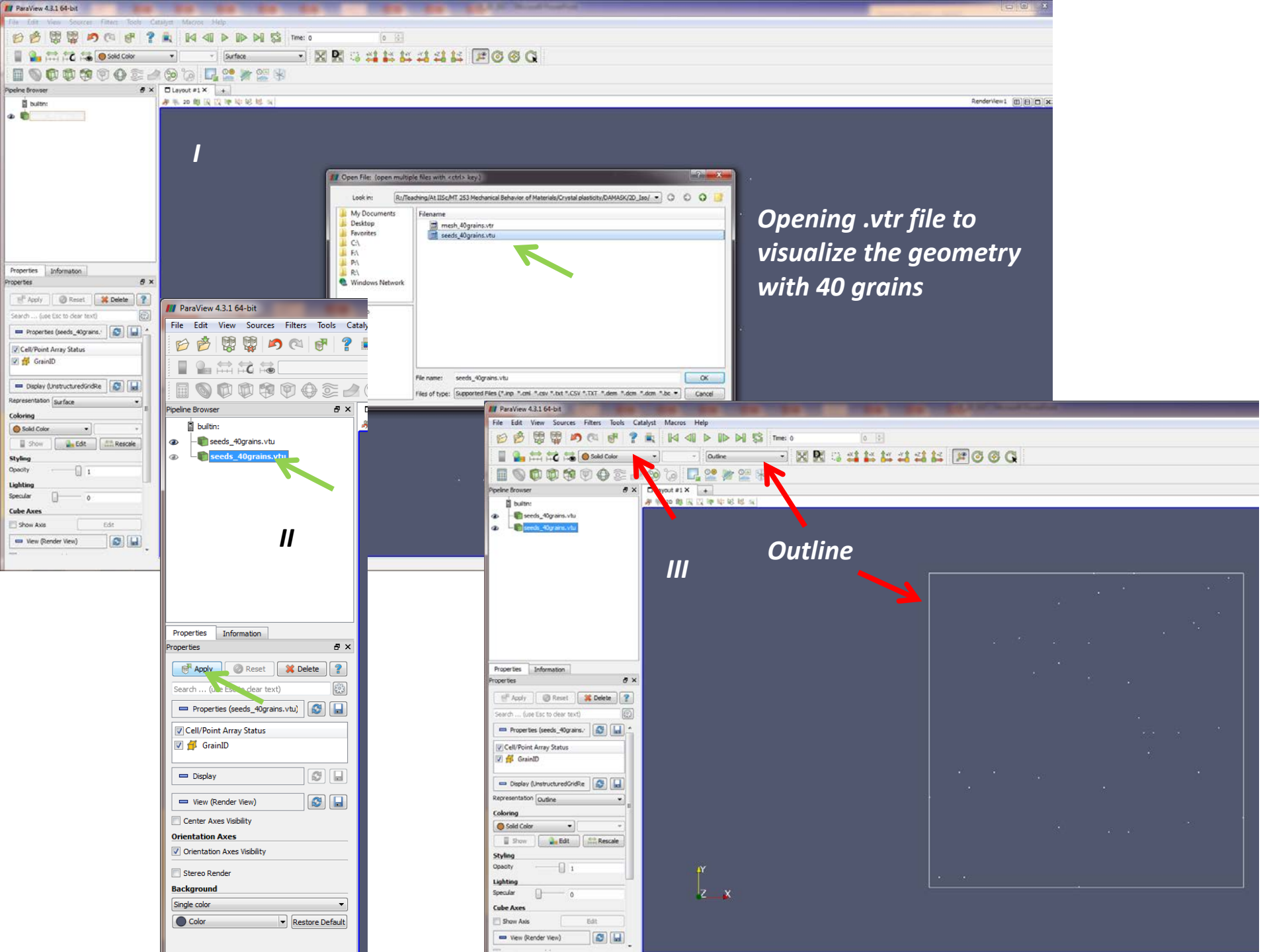
Transfer the files of interest to your machine for visualization using "paraview" or anything else

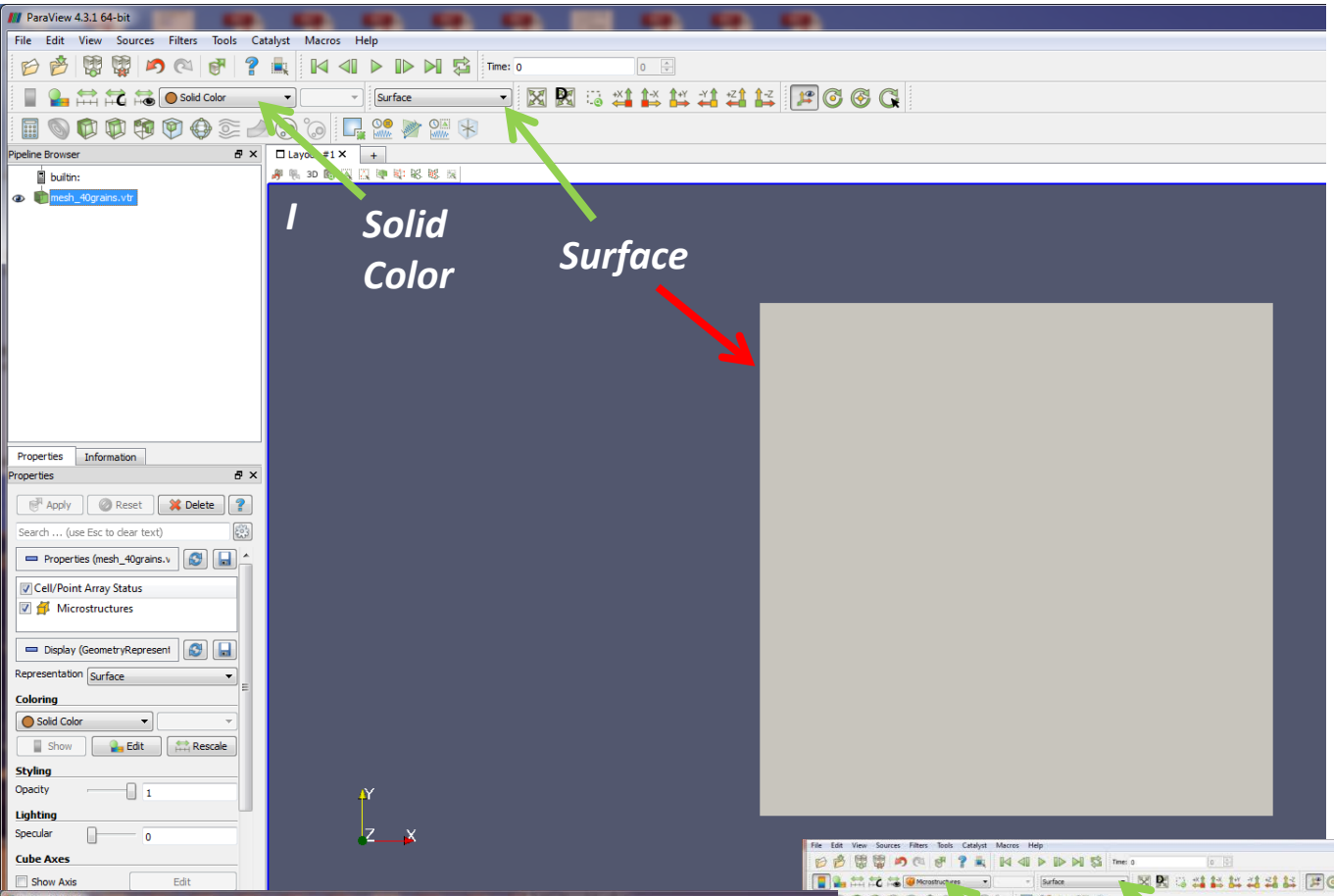
Open: Paraview Software

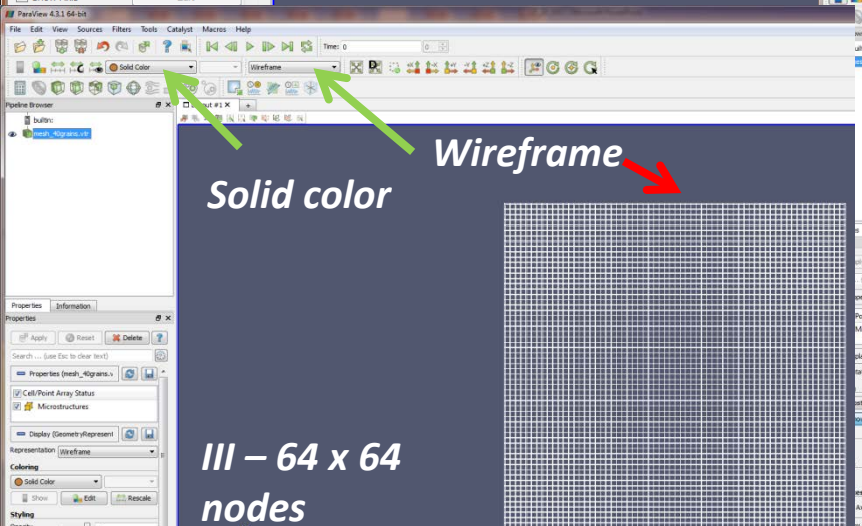
Opening .vtu file to visualize the positions of 40 points (pivot points for generating 40 grains)

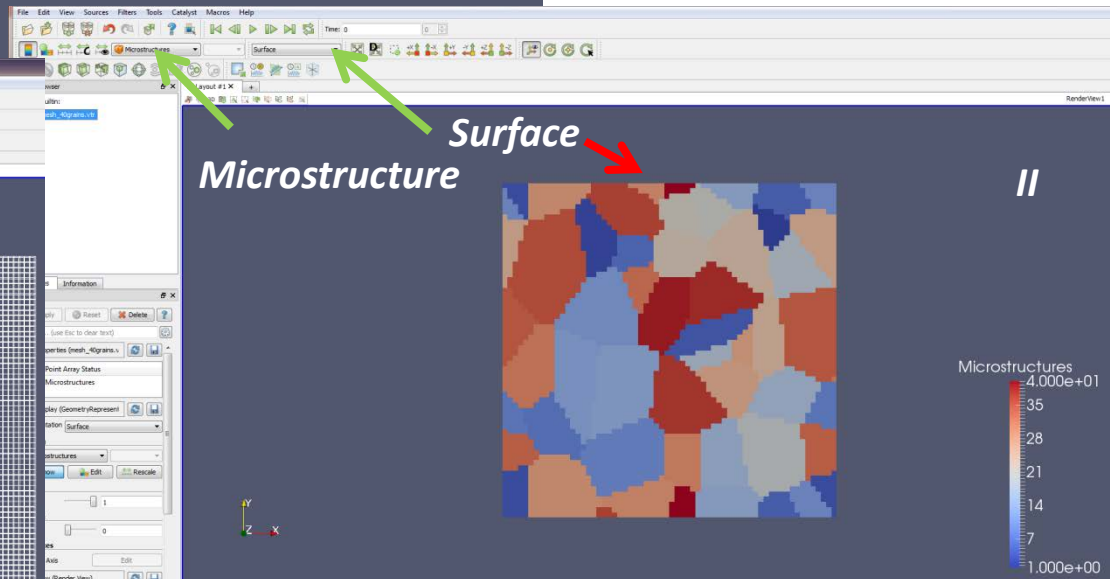


Locations of 40 points (positions are random – thus no two geometry created using the same commands will be same)


I
Opening .vtr file to visualize the geometry with 40 grains
II
III
Outline


I
Solid Color
Surface


Solid color
Wireframe
III – 64 x 64 nodes


Surface
Microstructure
II
Microstructures
4.000e+01
35
28
21
14
7
1.000e+00

```
[sandbox@materials25 PK01]$ geom_fromVoronoiTessellation --config 40grains.seeds

REMARK: h5py module not available

geom_fromVoronoiTessellation: 40grains.seeds
rescaling size x...
rescaling size y...
rescaling size z...
grains to map:  40
grid     a b c: 64 x 64 x 1
size     x y z: 1.0 x 1.0 x 0.015625
origin   x y z: 0.0 : 0.0 : 0.0
homogenization: 1
[sandbox@materials25 PK01]$ ll
total 36
-rw-r--r--. 1 sandbox users 12638 Jun 17 18:59 40grains.geom
-rw-r--r--. 1 sandbox users  6234 Jun 17 19:54 40grains_material.config
-rw-r--r--. 1 sandbox users  3287 Jun 17 18:58 40grains.seeds
-rw-r--r--. 1 sandbox users  2311 Jun 17 19:30 mesh_40grains.vtr
-rw-r--r--. 1 sandbox users  1751 Jun 17 19:29 seeds_40grains.vtu
[sandbox@materials25 PK01]$
[sandbox@materials25 PK01]$ cp 40grains_material.config material.config
[sandbox@materials25 PK01]$ ll
total 44
-rw-r--r--. 1 sandbox users 12638 Jun 17 18:59 40grains.geom
-rw-r--r--. 1 sandbox users  6234 Jun 17 19:54 40grains_material.config
-rw-r--r--. 1 sandbox users  3287 Jun 17 18:58 40grains.seeds
-rw-r--r--. 1 sandbox users  6234 Jun 17 19:57 material.config
-rw-r--r--. 1 sandbox users  2311 Jun 17 19:30 mesh_40grains.vtr
-rw-r--r--. 1 sandbox users  1751 Jun 17 19:29 seeds_40grains.vtu
[sandbox@materials25 PK01]$
```

Generates a configuration file consisting of details of materials geometry, such as …….

More on Voronoi Tessellation at:
https://en.wikipedia.org/wiki/Voronoi_diagram

Name of this file is first half of .seeds file followed by _material.config (which cannot be used by DAMASK program)

Copy (cp) the above file in a new file – "material.config" which will be used by DAMASK program

```
[sandbox@materials25 PK01]$ less material.config
#$Id: geom_fromVoronoiTessellation.py 4232M 2015-06-17 02:52:24Z (local) $ --config 40grains.seeds

<microstructure>

[Grain01]
crystallite 1
(constituent)   phase 1 texture  1      fraction 1.0

[Grain02]
crystallite 1
(constituent)   phase 1 texture  2      fraction 1.0

[Grain03]
crystallite 1
(constituent)   phase 1 texture  3      fraction 1.0

[Grain04]
crystallite 1
(constituent)   phase 1 texture  4      fraction 1.0

[Grain05]
crystallite 1
(constituent)   phase 1 texture  5      fraction 1.0

[Grain06]
crystallite 1
(constituent)   phase 1 texture  6      fraction 1.0

[Grain07]
crystallite 1
(constituent)   phase 1 texture  7      fraction 1.0

[Grain08]
crystallite 1
(constituent)   phase 1 texture  8      fraction 1.0

[Grain09]
crystallite 1
(constituent)   phase 1 texture  9      fraction 1.0

[Grain10]
crystallite 1
(constituent)   phase 1 texture 10      fraction 1.0

[Grain11]
crystallite 1
```

First <property>

First [Info for your reference – not used by program]

Reading "material.config" file (command "less"; enter or down-arrow to read below; "q" to exit

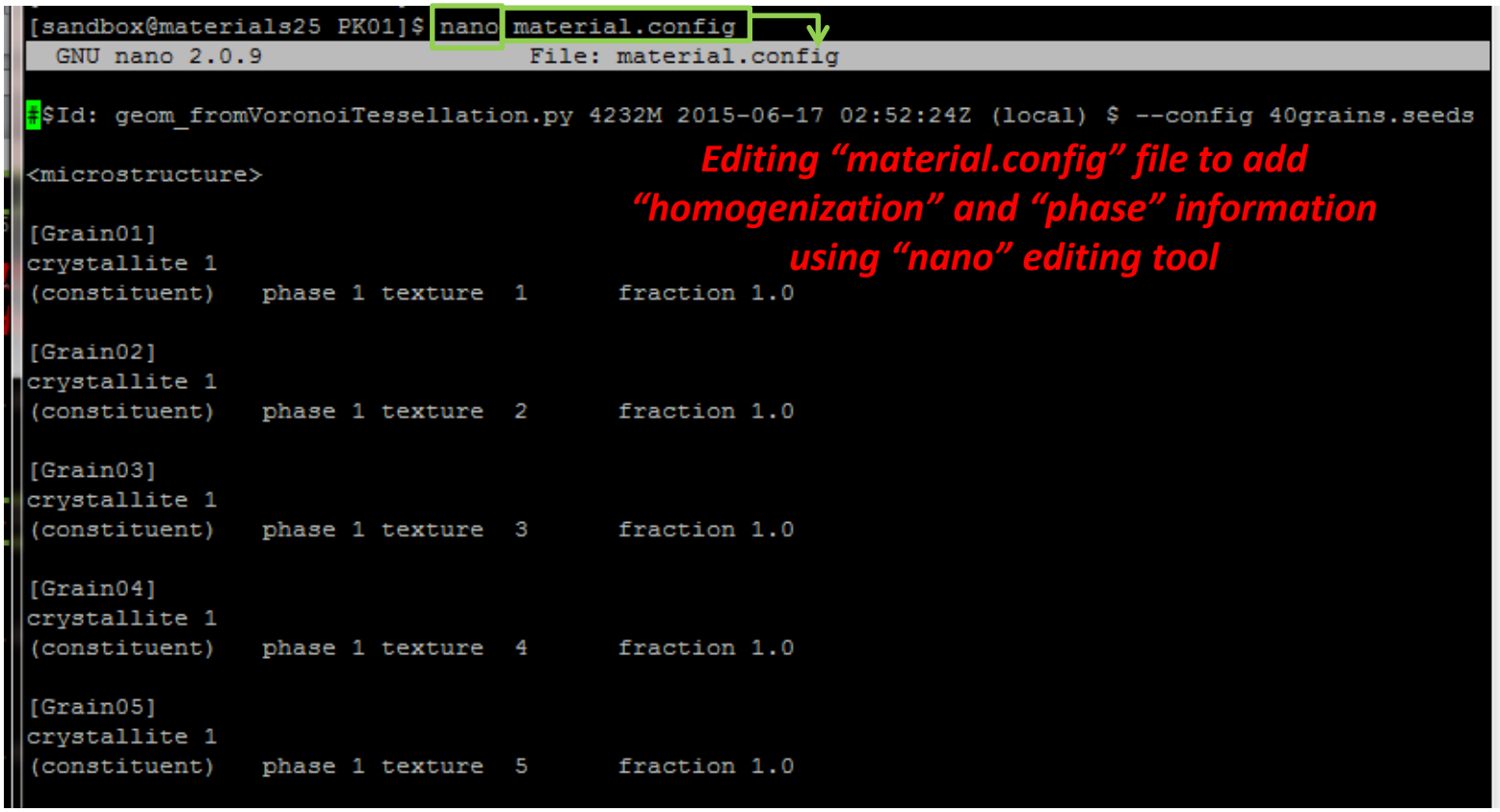
This crystallite has only one phase, only one but unique texture and this type of crystallite fills the entire region dedicated for this grain

→ The same thing for remaining 40 grains!

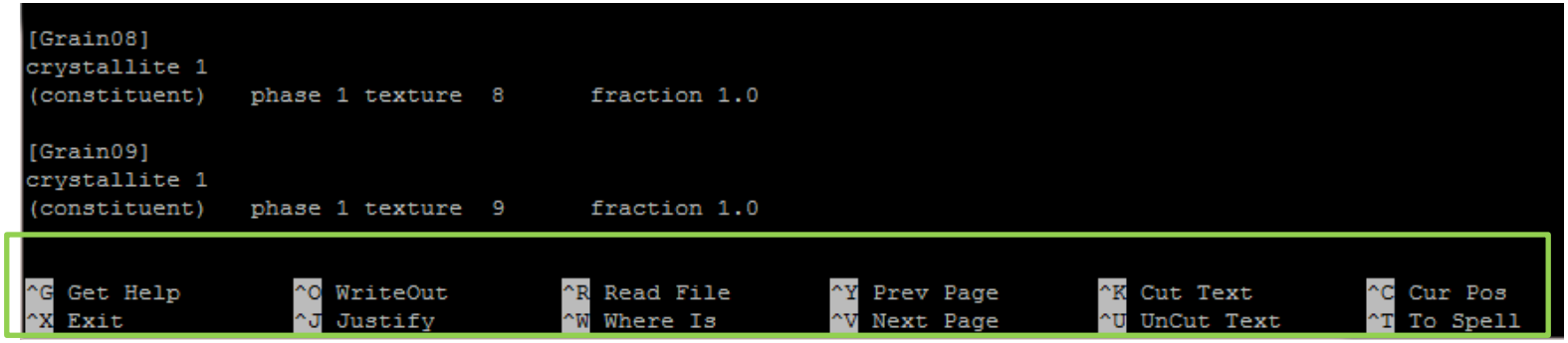
```
[Grain40]
crystallite 1
(constituent)   phase 1 texture 40      fraction 1.0

<texture>

[Grain01]
(gauss) phi1 85.4094    Phi 146.682     phi2 139.992    scatter 0.0     fraction 1.0

[Grain02]
(gauss) phi1 334.017    Phi 109.26      phi2 192.205    scatter 0.0     fraction 1.0

[Grain03]
(gauss) phi1 179.425    Phi 115.591     phi2 258.158    scatter 0.0     fraction 1.0

[Grain04]
(gauss) phi1 80.9573    Phi 107.351     phi2 0.478973   scatter 0.0     fraction 1.0

[Grain05]
(gauss) phi1 29.2884    Phi 89.2547     phi2 49.7917    scatter 0.0     fraction 1.0

[Grain06]
(gauss) phi1 243.364    Phi 149.049     phi2 202.51     scatter 0.0     fraction 1.0
```

Second <property>

Euler angles in ?? format



Editing "material.config" file to add "homogenization" and "phase" information using "nano" editing tool



Editing tools for "nano"

Saving a file (in "nano"):

1. *Ctrl + X to escape*
2. *Then "Y" to save the changes*
3. *"Enter" to keep the same name of the file (or change it by typing any name)*

```
#$Id: geom_fromVoronoiTessellation.py 4232M 2015-06-17 02:52:24Z (local) $ --config 40grains.seeds

<homogenization>
[SX]
type none

<crystallite>
[essential]
(output) texture
(output) f
(output) p
(output) orientation
(output) grainrotation

<microstructure>

[Grain01]
crystallite 1
(constituent)   phase 1 texture  1      fraction 1.0

[Grain02]
crystallite 1
(constituent)   phase 1 texture  2      fraction 1.0

[Grain03]
crystallite 1
(constituent)   phase 1 texture  3      fraction 1.0

[Grain04]
crystallite 1
(constituent)   phase 1 texture  4      fraction 1.0

[Grain05]
crystallite 1
(constituent)   phase 1 texture  5      fraction 1.0

[Grain06]
crystallite 1
(constituent)   phase 1 texture  6      fraction 1.0
```

Homogenization: there is only one type of homogenization – which is none!

Crystallite information:
[Essential] - name is just for your reference
Outputs of interest: texture, f (deformation gradient tensor), p (first Piola–Kirchhoff stress), orientation and grain rotation

```
^G Get Help   ^O WriteOut   ^R Read File   ^Y Prev Page   ^K Cut Text   ^C Cur Pos
^X Exit       ^J Justify    ^W Where Is    ^V Next Page   ^U UnCut Text ^T To Spell
```

```
#$Id: geom_fromVoronoiTessellation.py 4232M 2015-06-17 02:52:24Z (local) $ --config 40grains.seeds

<homogenization>
[SX]
type none

<crystallite>
[essential]
(output) texture
(output) f
(output) p
(output) orientation
(output) grainrotation

<phase>
{/opt/DAMASK/code/config/Phase_J2_AluminumIsotropic.config}

<microstructure>

[Grain01]
crystallite 1
(constituent)   phase 1 texture  1      fraction 1.0

[Grain02]
crystallite 1
(constituent)   phase 1 texture  2      fraction 1.0

[Grain03]
crystallite 1
(constituent)   phase 1 texture  3      fraction 1.0

[Grain04]
crystallite 1
(constituent)   phase 1 texture  4      fraction 1.0

[Grain05]
crystallite 1
(constituent)   phase 1 texture  5      fraction 1.0

[Grain06]

^G Get Help    ^O WriteOut    ^R Read File    ^Y Prev Page    ^K Cut Text    ^C Cur Pos
^X Exit        ^J Justify     ^W Where Is     ^V Next Page    ^U UnCut Text  ^T To Spell
```

Isotropic material

This is the routine (at /opt/… location)

```
[sandbox@materials25 config]$ cat Phase_J2_AluminumIsotropic.config
### $Id: Phase_J2_AluminumIsotropic.config 3824 2014-12-18 18:20:11Z MPIE\m.diehl $ ###
[Aluminum_Isotropic]
# Kuo, J. C., Mikrostrukturmechanik von Bikristallen mit Kippkorngrenzen. Shaker-Verlag 20
9

elasticity      hooke
plasticity      j2

(output) flowstress
(output) strainrate

lattice_structure isotropic

c11             110.9e9
c12             58.34e9
taylorfactor    3
tau0            31e6
gdot0           0.001
n               20
h0              75e6
tausat          63e6
w0              2.25
atol_resistance 1
[sandbox@materials25 config]$
```

Hookean elasticity

J2 plasticity (no hydrostatic stress effect)

Output – flow stress and strain rate

Stiffness tensor: C11 and C22 (isotropic)

tau0 – shear stress for slip on one plane, tausat – saturation stress, atol_resistance is a convergence parameter, and for other terms here, refer to next page (note w0 = a)

http://damask.mpie.de/Documentation/Isotropic

In accordance with the Peirce, Asaro, & Needleman (1983) law, the (average) shear rate is formulated as a power-law kinetic equation

$$\dot{\gamma} = \dot{\gamma}_0 \left(\frac{\sqrt{3 J_2}}{M\, g} \right)^n = \dot{\gamma}_0 \left(\sqrt{\frac{3}{2}} \frac{\|\mathbf{S}^*\|}{M\, g} \right)^n \tag{1}$$

$$\dot{\gamma} = \dot{\gamma}_0 \left(\frac{\sqrt{3 I_2}}{M\, g} \right)^n = \dot{\gamma}_0 \left(\sqrt{\frac{3}{2}} \frac{\|\mathbf{S}\|}{M\, g} \right)^n \tag{2}$$

with $\dot{\gamma}_0$ a reference shear rate, n the stress exponent (at constant structure), and M an orientation (Taylor) factor.

Structure

Again, following the hardening behavior suggested in Peirce, Asaro, & Needleman (1983), the flow stress g evolves in time due to deformation from its initial value g_0 towards a saturation value g_∞ according to

$$\dot{g} = \dot{\gamma} \left(h_0 + h_s \ln \dot{\gamma} \right) \left| 1 - g/g_\infty \right|^a \operatorname{sign} \left(1 - g/g_\infty \right), \tag{3}$$

with free parameters h_0 and a. The parameter $h_s = \mathrm{d}h_0 / \mathrm{d} \ln \dot{\gamma}$ introduces a strain rate sensitivity of the hardening slope.

To capture more than the power-law rate dependency of the saturation stress inherent in (1) and (2), we make use of the empirical relation

$$\begin{aligned} \dot{\gamma} &= A \left(\sinh \left(B\, g_\infty^* \right)^C \right)^D \\ &= A \left(\sinh \left(B\, g_\infty \left(\dot{\gamma} / \dot{\gamma}_0 \right)^{1/n} \right)^C \right)^D, \end{aligned} \tag{4}$$

where the factor $\left(\dot{\gamma} / \dot{\gamma}_0 \right)^{1/n}$ corrects the (experimentally observed) saturation stress g_∞^* for the rate sensitivity introduced by the deformation kinetics (1) and (2). Parameters A, B, C, and D allow for fitting.

The value of A is used to switch between constant saturation stress and rate-sensitive saturation behavior:

$$g_\infty = \begin{cases} \tau_{sat} & \text{if } A = 0 \\ \tau_{sat} + \left(\operatorname{asinh} \left(\left(\dot{\gamma} / A \right)^{1/D} \right) \right)^{1/C} \Big/ \left(B \left(\dot{\gamma} / \dot{\gamma}_0 \right)^{1/n} \right) & \text{otherwise} \end{cases} \tag{5}$$

sandbox@materials25:/opt/DAMASK/code/config

```
### $Id: Phase_Phenopowerlaw_Aluminum.config 4140 2015-05-05 20:17:50Z MPIE\m.diehl $ ###
[Aluminum]
elasticity              hooke
plasticity              phenopowerlaw

(output)                resistance_slip
(output)                shearrate_slip
(output)                resolvedstress_slip
(output)                accumulated_shear_slip
(output)                totalshear
(output)                resistance_twin
(output)                shearrate_twin
(output)                resolvedstress_twin
(output)                accumulated_shear_twin
(output)                totalvolfrac_twin

lattice_structure       fcc
Nslip                   12                  # per family
Ntwin                    0                  # per family

c11                     106.75e9
c12                     60.41e9
c44                     28.34e9

gdot0_slip              0.001
n_slip                  20
tau0_slip                 31e6              # per family
tausat_slip               63e6              # per family
a_slip                  2.25
gdot0_twin              0.001
n_twin                  20
tau0_twin                 31e6              # per family
s_pr                    0                   # push-up factor for slip saturation due to twinning
twin_b                  0
twin_c                  0
twin_d                  0
twin_e                  0
h0_slipslip             75e6
h0_twinslip             0
Phase_Phenopowerlaw_Aluminum.config
```

```
h0_twinslip             0
h0_twintwin             0
interaction_slipslip    1 1 1.4 1.4 1.4 1.4
interaction_sliptwin    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
interaction_twinslip    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
interaction_twintwin    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
atol_resistance         1
(END)
```

Instead of using "Isotropic material" option in <phase>, as follows

```
<phase>
{/opt/DAMASK/code/config/Phase_J2_AluminumIsotropic.config}
```

One may also use the following for describing material plasticity: a bit more realistic choice:

<phase>
{/opt/DAMASK/code/config/Phase_Phenopowerlaw_Aluminum.config}

This is the routine (at /opt/… location)

To define load file – let's use "nano" command to create a file called "tensionY.load"

sandbox@materials25:~/praveenk/PK01

```
 GNU nano 2.0.9                File: tensionY.load

Fdot * 0 0 0 1e-3 0 0 0 0 stress 0 * * * * * * * * time 100 incs 200 freq 5
```

I

1. * represents unconstrained BC
2. Strain rate in y direction is 10^{-3} s^{-1}
3. Stress in x-direction must be zero (traction free)
4. Load it for 100 seconds (i.e., up to 0.1 strain)
5. Total increments to finish is 200 (i.e. each time step is of 0.5 seconds)
6. Save data with frequency of 5 – so total 40 sets of data will be saved

More than one loading sequence can be applied by writing "all loading /boundary conditions commands" in different lines (first line is first set of loading, etc.)

II

```
[sandbox@materials25 PK01]$ ll
total 48
-rw-r--r--. 1 sandbox users 12638 Jun 17 18:59 40grains.geom
-rw-r--r--. 1 sandbox users  6234 Jun 17 19:54 40grains_material.config
-rw-r--r--. 1 sandbox users  3287 Jun 17 18:58 40grains.seeds
-rw-r--r--. 1 sandbox users  6446 Jun 17 20:25 material.config
-rw-r--r--. 1 sandbox users  2311 Jun 17 19:30 mesh_40grains.vtr
-rw-r--r--. 1 sandbox users  1751 Jun 17 19:29 seeds_40grains.vtu
-rw-r--r--. 1 sandbox users    82 Jun 17 20:55 tensionY.load
[sandbox@materials25 PK01]$
```

sandbox@materials25:~/praveenk/PK01

```
 GNU nano 2.0.9                File: tensionY.load

Fdot   * 0 0 0 1e-3 0 0 0 0
stress 0 * * *  *   * * * *
time 100 incs 200
freq 5

^G Get Help    ^O WriteOut    ^R Read File   ^Y Prev Page   ^K Cut Text    ^C Cur Pos
^X Exit        ^J Justify     ^W Where Is    ^V Next Page   ^U UnCut Text  ^T To Spell
```

Do not write it with "new lines"

```
[sandbox@materials25 PK01]$ DAMASK_spectral --load tensionY.load --geom 40grains.geom > 40grains_tensionY.out &
[1] 31787
[sandbox@materials25 PK01]$
```

Job number at "server" computer

Run simulation (DAMASK software, Spectral method)

Using these load and geometry

Write solution in this file

Run in background

I

```
[sandbox@materials25 PK01]$ ll
total 47004
-rw-r--r--. 1 sandbox users    12638 Jun 17 18:59 40grains.geom
-rw-r--r--. 1 sandbox users     6234 Jun 17 19:54 40grains_material.config
-rw-r--r--. 1 sandbox users     3287 Jun 17 18:58 40grains.seeds
-rw-r--r--. 1 sandbox users      648 Jun 17 21:06 40grains_tensionY.C_ref
-rw-r--r--. 1 sandbox users  1100085 Jun 17 21:06 40grains_tensionY_ipbased.vtk
-rw-r--r--. 1 sandbox users  1005058 Jun 17 21:06 40grains_tensionY.mesh
-rw-r--r--. 1 sandbox users  1100088 Jun 17 21:06 40grains_tensionY_nodebased.vtk
-rw-r--r--. 1 sandbox users   496515 Jun 17 21:14 40grains_tensionY.out
-rw-r--r--. 1 sandbox users       71 Jun 17 21:06 40grains_tensionY.outputConstitutive
-rw-r--r--. 1 sandbox users       77 Jun 17 21:06 40grains_tensionY.outputCrystallite
-rw-r--r--. 1 sandbox users      148 Jun 17 21:06 40grains_tensionY.outputHomogenization
-rw-r--r--. 1 sandbox users 44335461 Jun 17 21:14 40grains_tensionY.spectralOut
-rw-r--r--. 1 sandbox users    13055 Jun 17 21:14 40grains_tensionY.sta
-rw-r--r--. 1 sandbox users     6446 Jun 17 20:25 material.config
-rw-r--r--. 1 sandbox users     2311 Jun 17 19:30 mesh_40grains.vtr
-rw-r--r--. 1 sandbox users     1751 Jun 17 19:29 seeds_40grains.vtu
-rw-r--r--. 1 sandbox users       76 Jun 17 21:05 tensionY.load
[sandbox@materials25 PK01]$
```

Also important files

II

```
[sandbox@materials25 PK01]$ cat *sta
Increment Time CutbackLevel Converged IterationsNeeded
        1  0.5000000000000000               0 T               1
        2   1.000000000000000               0 T               1
        3   1.500000000000000               0 T               1
        4   2.000000000000000               0 T               1
        5   2.500000000000000               0 T               1
        6   3.000000000000000               0 T               1
        7   3.500000000000000               0 T               1
        8   4.000000000000000               0 T               1
```

III

*"cat" or "less" 40grains_tensionY.sta or *.sta file (as its only one in there of this type – "*" subsitutes for the probable file names in folder)*

For this simple problem, it converges in 1 step itself (more on next slide)

"tail" 40grains_tensionY.out to check the progress

```
[sandbox@materials25 PK01]$ tail -f 40grains_tensionY.out
```

sandbox@materials25:~/praveenk/PK01

```
... reporting .....................................................

error divergence =          0.00 (1.53E-04 / m, tol = 5.87E+04)
error stress BC =           2.23 (2.62E+06 Pa,  tol = 1.17E+06)

================================================================

Increment 5/200-1/1 @ Iteration 001≤001≤250

deformation gradient aim =
  0.9982233     0.0000000     0.0000000
  0.0000000     1.0025000     0.0000000
  0.0000000     0.0000000     1.0000000

... evaluating constitutive response ..............................

Piola--Kirchhoff stress / MPa =
       0.0297        0.0000       -0.0000
       0.0000      115.0748        0.0000
      -0.0000        0.0000       49.0089

... calculating divergence ........................................

... doing gamma convolution .......................................

... evaluating constitutive response ..............................

Piola--Kirchhoff stress / MPa =
       0.0000       -0.0000        0.0000
      -0.0000      115.0476        0.0000
       0.0000        0.0000       48.9875

... calculating divergence ........................................

... doing gamma convolution .......................................

... reporting .....................................................

error divergence =          0.00 (4.73E-05 / m, tol = 5.75E+04)
error stress BC =           0.00 (4.13E+01 Pa,  tol = 1.15E+06)

================================================================

increment 5 converged

... writing results to file .......................................

############################################################################
Time 3.00000E+00s: Increment 6/200-1/1 of load case 1/1
Increment 6/200-1/1 @ Iteration 001≤000≤250

deformation gradient aim =
  0.9977466     0.0000000     0.0000000
  0.0000000     1.0030000     0.0000000
  0.0000000     0.0000000     1.0000000

... evaluating constitutive response ..............................
```

I

5th out of 200 steps

At one step

Next iteration value for the stress tensor – and it actually converges (i.e., satisfies atol_resistance criterion) in one step itself

```
================================================================

increment 200 converged
STOP 0

... writing results to file .......................................

############################################################################
000200 out of 000200 (100.0 %) increments converged!

DAMASK terminated on:
Date:                17/06/2015
Time:                21:14:17
```

Simulation run finishes

II

"Ctrl + C" to finish "tail"

Creates a folder postProc with text file containing "average of all load steps" f and p results (no time resolution here)

sandbox@materials25:~/praveenk/PK01

```
[sandbox@materials25 PK01]$ postResults 40grains_tensionY.spectralOut --cr f,p

REMARK: h5py module not available

(00:01:39) processing point 1000 of 4096 from increment 5 (position 1)...
```

-- cr (crystallite outputs → check in .config file for options) Write – f and p

I

```
[sandbox@materials25 PK01]$ postResults 40grains_tensionY.spectralOut --cr f,p

REMARK: h5py module not available

andbox@materials25 PK01]$ ll
total 47008
-rw-r--r--. 1 sandbox users    12638 Jun 17 18:59 40grains.geom
-rw-r--r--. 1 sandbox users     6234 Jun 17 19:54 40grains_material.config
-rw-r--r--. 1 sandbox users     3287 Jun 17 18:58 40grains.seeds
-rw-r--r--. 1 sandbox users      648 Jun 17 21:06 40grains_tensionY.C_ref
-rw-r--r--. 1 sandbox users  1100085 Jun 17 21:06 40grains_tensionY_ipbased.vtk
-rw-r--r--. 1 sandbox users  1005058 Jun 17 21:06 40grains_tensionY.mesh
-rw-r--r--. 1 sandbox users  1100088 Jun 17 21:06 40grains_tensionY_nodebased.vtk
-rw-r--r--. 1 sandbox users   496515 Jun 17 21:14 40grains_tensionY.out
-rw-r--r--. 1 sandbox users       71 Jun 17 21:06 40grains_tensionY.outputConstitutive
-rw-r--r--. 1 sandbox users       77 Jun 17 21:06 40grains_tensionY.outputCrystallite
-rw-r--r--. 1 sandbox users      148 Jun 17 21:06 40grains_tensionY.outputHomogenization
-rw-r--r--. 1 sandbox users 44335461 Jun 17 21:14 40grains_tensionY.spectralOut
-rw-r--r--. 1 sandbox users    13055 Jun 17 21:14 40grains_tensionY.sta
-rw-r--r--. 1 sandbox users     6446 Jun 17 20:25 material.config
-rw-r--r--. 1 sandbox users     2311 Jun 17 19:30 mesh_40grains.vtr
drwxr-xr-x. 2 sandbox users     4096 Jun 17 21:27 postProc
-rw-r--r--. 1 sandbox users     1751 Jun 17 19:29 seeds_40grains.vtu
-rw-r--r--. 1 sandbox users       76 Jun 17 21:05 tensionY.load
[sandbox@materials25 PK01]$ cd postProc
[sandbox@materials25 postProc]$ ll
total 16
-rw-r--r--. 1 sandbox users 12346 Jun 17 21:29 40grains_tensionY.txt
```

Change directory (cd) to postProc and then long list items in there

II

sandbox@materials25:~/praveenk/PK01/postProc

```
[sandbox@materials25 postProc]$ pwd
/home/sandbox/praveenk/PK01/postProc
[sandbox@materials25 postProc]$ showTable --label 40grains_tensionY.txt

REMARK: h5py module not available

showTable: 40grains_tensionY.txt
inc     elem    node    ip      grain   1_ipinitialcoord        2_ipinitialcoord        3_ipinitialcoord        1_f_2
 f      3_f     4_f     5_f     6_f     7_f     8_f     9_f     1_p     2_p     3_p     4_p     5_p     6_p     7_p_8
_p      9_p
[sandbox@materials25 postProc]$
```

Working directory (pwd)

showTable (shows table), showTable --abc
Shows a component of the table

Txt file has all data in table with these "labels"

2-D tensors of f and p are written row-wise → so a_{xy} is (2*(x-1)+y)_a

I

```
_p      9_p
[sandbox@materials25 postProc]$ addStrainTensors 40grains_tensionY.txt --left --logarithmic

REMARK: h5py module not available

addStrainTensors: 40grains_tensionY.txt
[sandbox@materials25 postProc]$ showTable --label 40grains_tensionY.txt

REMARK: h5py module not available

showTable: 40grains_tensionY.txt
inc     elem    node    ip      grain   1_ipinitialcoord        2_ipinitialcoord        3_ipinitialcoord        1_f     2_f     3_f     4_f     5_f     6_f     7_f
8_f     9_f     1_p     2_p     3_p     4_p     5_p     6_p     7_p     8_p     9_p     1_ln(V) 2_ln(V) 3_ln(V) 4_ln(V) 5_ln(V) 6_ln(V) 7_ln(V) 8_ln(V) 9_ln(V)
[sandbox@materials25 postProc]$
```

II

Add (Left Cauchy-Green) strain tensor in table from the displacement gradient tensor

--left (left strain tensor), --logarithmic (true strain)

```
[sandbox@materials25 postProc]$ addCauchy 40grains_tensionY.txt

REMARK: h5py module not available

addCauchy: 40grains_tensionY.txt
[sandbox@materials25 postProc]$ showTable --label 40grains_tensionY.txt

REMARK: h5py module not available

showTable: 40grains_tensionY.txt
inc     elem    node    ip      grain   1_ipinitialcoord        2_ipinitialcoord        3_ipinitialcoord        1_f     2_f     3_f     4_f     5_f     6_f
_f      9_f     1_p     2_p     3_p     4_p     5_p     6_p     7_p     8_p     9_p     1_ln(V) 2_ln(V) 3_ln(V) 4_ln(V) 5_ln(V) 6_ln(V) 7_ln(V) 8_ln(V) 9_ln(V)
uchy    2_Cauchy        3_Cauchy        4_Cauchy        5_Cauchy        6_Cauchy        7_Cauchy        8_Cauchy        9_Cauchy
[sandbox@materials25 postProc]$
```

III

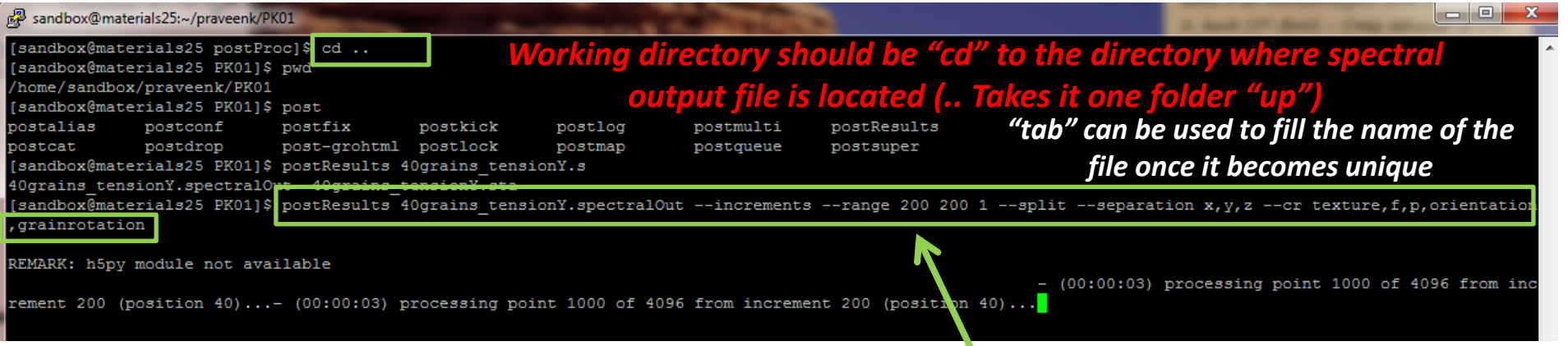
Add (calculate) Cauchy stress tensor from first Piola-Kirchhoff stress tensor

```
[sandbox@materials25 postProc]$ addMises 40grains_tensionY.txt --strain 'ln(V)' stress Cauchy

REMARK: h5py module not available

addMises: 40grains_tensionY.txt
[sandbox@materials25 postProc]$ showTable --label 40grains_tensionY.txt

REMARK: h5py module not available

showTable: 40grains_tensionY.txt
inc     elem    node    ip      grain   1_ipinitialcoord        2_ipinitialcoord        3_ipinitialcoord        1_f     2_f     3_f     4_f     5_f     6_f     7_
_f      9_f     1_p     2_p     3_p     4_p     5_p     6_p     7_p     8_p     9_p     1_ln(V) 2_ln(V) 3_ln(V) 4_ln(V) 5_ln(V) 6_ln(V) 7_ln(V) 8_ln(V) 9_ln(V) 1_
uchy    2_Cauchy        3_Cauchy        4_Cauchy        5_Cauchy        6_Cauchy        7_Cauchy        8_Cauchy        9_Cauchy        Mises(ln(V))
[sandbox@materials25 postProc]$
```

IV

Generate Mises strain using Left Cauchy-Green Strain and Cauchy Stress Tensors and Add it to table

Spectrally resolved data → data at each time increment (unlike the average we got in the last slide)



Working directory should be "cd" to the directory where spectral output file is located (.. Takes it one folder "up")

"tab" can be used to fill the name of the file once it becomes unique

Note: (i) need for defining increments and range of data – 200 is total number of steps but we are interested in only the last step (200th), (ii) get it by splitting the data set, (iii) identify each data point from its x,y,z coordinates, and (iv) produce crystallite outputs of f, p, etc.

Following generation of a new text file in postProc folder (with a name ending with _inc200.txt) (_inc200 here means the data achieved at 200th increment – i.e., the last step), we again need to generate strain tensors, Cauchy stress tensor and the finally Mises strain following the same procedure as described before and shown in next slide.

sandbox@materials25:~/praveenk/PK01/postProc

```
[sandbox@materials25 PK01]$ ll
total 47008
-rw-r--r--. 1 sandbox users    12638 Jun 17 18:59 40grains.geom
-rw-r--r--. 1 sandbox users     6234 Jun 17 19:54 40grains_material.config
-rw-r--r--. 1 sandbox users     3287 Jun 17 18:58 40grains.seeds
-rw-r--r--. 1 sandbox users      648 Jun 17 21:06 40grains_tensionY.C_ref
-rw-r--r--. 1 sandbox users  1100085 Jun 17 21:06 40grains_tensionY_ipbased.vtk
-rw-r--r--. 1 sandbox users  1005058 Jun 17 21:06 40grains_tensionY.mesh
-rw-r--r--. 1 sandbox users  1100088 Jun 17 21:06 40grains_tensionY_nodebased.vtk
-rw-r--r--. 1 sandbox users   496515 Jun 17 21:14 40grains_tensionY.out
-rw-r--r--. 1 sandbox users       71 Jun 17 21:06 40grains_tensionY.outputConstitutive
-rw-r--r--. 1 sandbox users       77 Jun 17 21:06 40grains_tensionY.outputCrystallite
-rw-r--r--. 1 sandbox users      148 Jun 17 21:06 40grains_tensionY.outputHomogenization
-rw-r--r--. 1 sandbox users 44335461 Jun 17 21:14 40grains_tensionY.spectralOut
-rw-r--r--. 1 sandbox users    13055 Jun 17 21:14 40grains_tensionY.sta
-rw-r--r--. 1 sandbox users     6446 Jun 17 20:25 material.config
-rw-r--r--. 1 sandbox users     2311 Jun 17 19:30 mesh_40grains.vtr
drwxr-xr-x. 2 sandbox users     4096 Jun 17 21:56 postProc
-rw-r--r--. 1 sandbox users     1751 Jun 17 19:29 seeds_40grains.vtu
-rw-r--r--. 1 sandbox users       76 Jun 17 21:05 tensionY.load
[sandbox@materials25 PK01]$ cd postProc
[sandbox@materials25 postProc]$ ll
total 1588
-rw-r--r--. 1 sandbox users 1598991 Jun 17 21:57 40grains_tensionY_inc200.txt
-rw-r--r--. 1 sandbox users   22731 Jun 17 21:48 40grains_tensionY.txt
[sandbox@materials25 postProc]$ addMises 40grains_tensionY_inc200.txt --strain 'ln(V)' --stress Cauchy

REMARK: h5py module not available

addStrainTensors: 40grains_tensionY_inc200.txt
[sandbox@materials25 postProc]$ addCauchy 40grains_tensionY_inc200.txt

REMARK: h5py module not available

addCauchy: 40grains_tensionY_inc200.txt
[sandbox@materials25 postProc]$ add Mises 40grains_tensionY_inc200.txt 'ln(V)' --stress Cauchy
-bash: add: command not found
[sandbox@materials25 postProc]$ addMises 40grains_tensionY_inc200.txt 'ln(V)' --stress Cauchy

REMARK: h5py module not available

addMises: 40grains_tensionY_inc200.txt
[sandbox@materials25 postProc]$
```

I

New file with "new" table

Old file remains there

```
[sandbox@materials25 postProc]$ showTable --label 40grains_tensionY_inc200.txt

REMARK: h5py module not available

showTable: 40grains_tensionY_inc200.txt
inc  elem  node  ip  grain  1_ipinitialcoord  2_ipinitialcoord  3_ipinitialcoord  texture  1_f  2_f  3_f  4_f  5_f6
_f  7_f  8_f  9_f  1_p  2_p  3_p  4_p  5_p  6_p  7_p  8_p  9_p  1_orientation  2_orientation  3_orientation  4_or
ientation  1_grainrotation  2_grainrotation  3_grainrotation  4_grainrotation  1_ln(V)  2_ln(V)  3_ln(V)  4_ln(V)  5_ln(V)  6_ln(V)  7_ln(V)  8_ln(V)  9_ln(V)  1_Ca
uchy  2_Cauchy  3_Cauchy  4_Cauchy  5_Cauchy  6_Cauchy  7_Cauchy  8_Cauchy  9_Cauchy  Mises(Cauchy)
[sandbox@materials25 postProc]$
```

II

: Mises(ln(V))

```
[sandbox@materials25 postProc]$ addIPFcolor 40grains_tensionY_inc200.txt --pole 0 0 1 --symmetry cubic --quaternion orientation

REMARK: h5py module not available

addIPFcolor: 40grains_tensionY_inc200.txt
[sandbox@materials25 postProc]$
```

Inverse pole figures with (001) pole in cubic system

```
[sandbox@materials25 postProc]$ showTable --label 40grains_tensionY_inc200.txt

REMARK: h5py module not available

showTable: 40grains_tensionY_inc200.txt
inc     elem    node    ip      grain   1_ipinitialcoord        2_ipinitialcoord        3_ipinitialcoord  t
exture  1_f     2_f     3_f     4_f     5_f     6_f     7_f     8_f     9_f     1_p     2_p     3_p     4_p
5_p     6_p     7_p     8_p     9_p     1_orientation   2_orientation   3_orientation   4_orientation   1_g
rainrotation    2_grainrotation 3_grainrotation 4_grainrotation 1_ln(V) 2_ln(V) 3_ln(V) 4_ln(V) 5_ln(V) 6_l
n(V)    7_ln(V) 8_ln(V) 9_ln(V) 1_Cauchy        2_Cauchy        3_Cauchy        4_Cauchy        5_Cauchy  6
_Cauchy 7_Cauchy        8_Cauchy        9_Cauchy        Mises(Cauchy)   1_IPF_001_cubic 2_IPF_001_cubic 3_I
PF_001_cubic    Mises(ln(V))    Mises(Cauchy)
[sandbox@materials25 postProc]$
```

```
[sandbox@materials25 postProc]$ imageDataRGB 40grains_tensionY_inc200.txt --label IPF_001_cubic --dimension 64 64

REMARK: h5py module not available

imageDataRGB: 40grains_tensionY_inc200.txt
[sandbox@materials25 postProc]$ ll
total 2804
-rw-r--r--. 1 sandbox users    1577 Jun 17 22:36 40grains_tensionY_inc200_IPF_001_cubic.png
-rw-r--r--. 1 sandbox users       0 Jun 17 22:34 40grains_tensionY_inc200_Mises(ln(V)).png
-rw-r--r--. 1 sandbox users 2839931 Jun 17 22:26 40grains_tensionY_inc200.txt
-rw-r--r--. 1 sandbox users   22731 Jun 17 21:48 40grains_tensionY.txt
[sandbox@materials25 postProc]$
```

Produces an image with "RGB" colours

Take data from time table under given lable

Dimension of data is 64 x 64

Transfer it to your computer from server computer for viewing

postProc - sandbox@10.194.30.25 - WinSCP

Local Mark Files Commands Session Options Remote Help

Default

R: Data

R:\Teaching\At IISc\MT 253 Mechanical Behavior of Materials\Crystal plasticity\DAMASK\2D_Iso

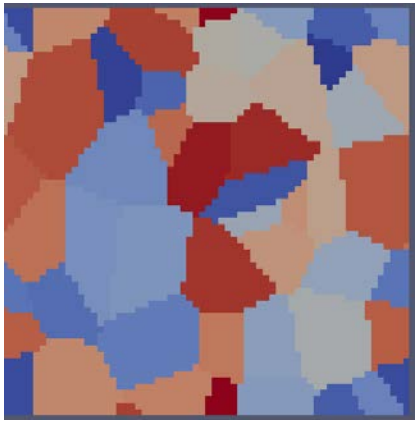
Name	Ext	Size	Type	Changed	Attr
..			Parent directory	17-Jun-2015 10:37:56 PM	
40grains.geom		12,638	GEOM File	17-Jun-2015 6:59:19 PM	a
40grains_tensionY_inc200_Mises(ln(V)).png		0	PNG image	17-Jun-2015 10:19:56 PM	a
40grains.seeds		3,287	SEEDS File	17-Jun-2015 6:58:25 PM	a
mesh_40grains.vtr		2,311	VTR File	17-Jun-2015 7:30:00 PM	a
seeds_40grains.vtu		1,751	VTU File	17-Jun-2015 7:29:35 PM	a

postProc

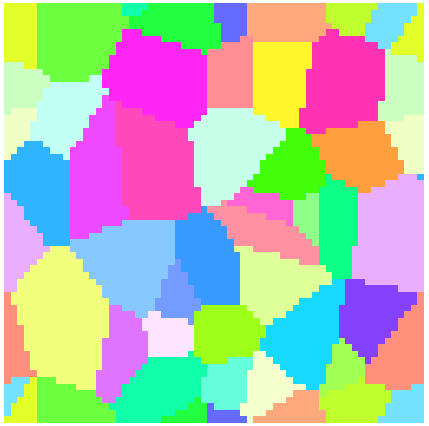
/home/sandbox/praveenk/PK01/postProc

Name	Ext	Size	Changed	Rights	Owner
..			17-Jun-15 9:27:56 PM	rwxr-xr-x	sandbox
40grains_tensionY_inc200_IPF_001_cubic.png		1,577	17-Jun-15 10:36:02 PM	rw-r--r--	sandbox
40grains_tensionY_inc200_Mises(ln(V)).png		0	17-Jun-15 10:34:59 PM	rw-r--r--	sandbox
40grains_tensionY.txt		22,731	17-Jun-15 9:48:50 PM	rw-r--r--	sandbox
40grains_tensionY_inc200.txt		2,839,931	17-Jun-15 10:26:02 PM	rw-r--r--	sandbox

Initial Geometry



IPF after loading



-1,577 B of 19,987 B in 0 of 5

1,577 B of 2,797 KiB in 1 of 4

F2 Rename F4 Edit F5 Copy F6 Move F7 Create Directory F8 Delete F9 Properties F10 Quit

SFTP-3 3:00:04

sandbox@materials25:~/praveenk/PK01/postProc

```
[sandbox@materials25 postProc]$ ll
total 2804
-rw-r--r--. 1 sandbox users    1577 Jun 17 22:36 40grains_tensionY_inc200_IPF_001_cubic.png
-rw-r--r--. 1 sandbox users 2839931 Jun 19 16:53 40grains_tensionY_inc200.txt
-rw-r--r--. 1 sandbox users   22731 Jun 17 21:48 40grains_tensionY.txt
[sandbox@materials25 postProc]$ imageData 40grains_tensionY_inc200.txt --label 'Mises(ln(V))' --dimension 64 64
imageData: 40grains_tensionY_inc200.txt
data range: 0.109545 -- 0.109545
1.00000563386e-12 0.109545416316 9.12868532049e-12
[sandbox@materials25 postProc]$ ll
total 2808
-rw-r--r--. 1 sandbox users    1577 Jun 17 22:36 40grains_tensionY_inc200_IPF_001_cubic.png
-rw-r--r--. 1 sandbox users     153 Jun 23 18:56 40grains_tensionY_inc200_Mises(ln(V)).png
-rw-r--r--. 1 sandbox users 2839931 Jun 19 16:53 40grains_tensionY_inc200.txt
-rw-r--r--. 1 sandbox users   22731 Jun 17 21:48 40grains_tensionY.txt
[sandbox@materials25 postProc]$
```

Produces an image

Take data from time table under given lable

Dimension of data is 64 x 64

Transfer it to your computer from server computer for viewing

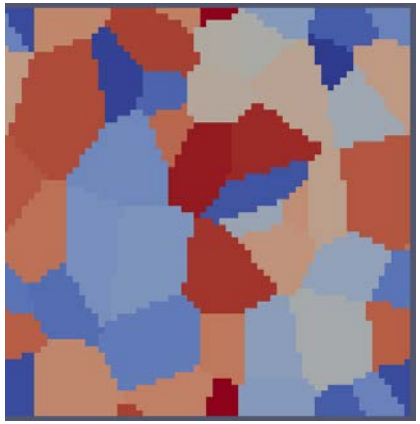
Local Mark Files Commands Session Options Remote Help

R: Data

R:\Teaching\At IISc\MT 253 Mechanical Behavior of Materials\Crystal plasticity\DAMASK\2D_Iso\PK01\postProc

Name	Ext	Size	Type	Changed	Attr
..			Parent directory	23-Jun-2015 7:07:23 PM	
40grains_tensionY_inc200_IPF_001_cubic.png		1,577	PNG image	17-Jun-2015 10:36:02 PM	a
40grains_tensionY_inc200_Mises(ln(V)).png		153	PNG image	23-Jun-2015 6:56:29 PM	a
40grains_tensionY.txt		22,778	Text Document	17-Jun-2015 9:48:50 PM	a
40grains_tensionY_inc200.txt		2,844,035	Text Document	19-Jun-2015 4:53:09 PM	a

Initial Geometry



postProc

/home/sandbox/praveenk/PK01/postProc

Name	Ext	Size	Changed	Rights	Owner
..			17-Jun-15 9:27:56 PM	rwxr-xr-x	sandbox
40grains_tensionY_inc200_IPF_001_cubic.png		1,577	17-Jun-15 10:36:02 PM	rw-r--r--	sandbox
40grains_tensionY_inc200_Mises(ln(V)).png		153	23-Jun-15 6:56:29 PM	rw-r--r--	sandbox
40grains_tensionY.txt		22,731	17-Jun-15 9:48:50 PM	rw-r--r--	sandbox
40grains_tensionY_inc200.txt		2,839,931	19-Jun-15 4:53:09 PM	rw-r--r--	sandbox

Note: No "--color bluered" command in "imageData", so plot is in greyscale

Von Mises strain after loading

(in isotropic material under unixial tension, von Mises strain is constant/uniform – not so interesting!)

0 B of 2,801 KiB in 0 of 4

153 B of 2,797 KiB in 1 of 4

Tutorial 2: Uniaxial tension type loading on a crystalline material (specific slip systems, etc.)

Make a new directory (in this case PK_02), go there and copy geometry, configuration, visualization (vtu & vtr) and load files from praveenk/PK_01 to this directory

```
[sandbox@materials25 PK02]$ pwd
/home/sandbox/praveenk/PK02
[sandbox@materials25 PK02]$ cp ../PK01/40grains.geom .
[sandbox@materials25 PK02]$ ll
total 16
-rw-r--r--. 1 sandbox users 12638 Jun 24 14:19 40grains.geom
[sandbox@materials25 PK02]$ cp ../PK01/material.config .
[sandbox@materials25 PK02]$ ll
total 24
-rw-r--r--. 1 sandbox users 12638 Jun 24 14:19 40grains.geom
-rw-r--r--. 1 sandbox users  6446 Jun 24 14:20 material.config
[sandbox@materials25 PK02]$ cp ../PK01/*.v* .
[sandbox@materials25 PK02]$ ll
total 2184
-rw-r--r--. 1 sandbox users   12638 Jun 24 14:19 40grains.geom
-rw-r--r--. 1 sandbox users 1100085 Jun 24 14:22 40grains_tensionY_ipbased.vtk
-rw-r--r--. 1 sandbox users 1100088 Jun 24 14:22 40grains_tensionY_nodebased.vtk
-rw-r--r--. 1 sandbox users    6446 Jun 24 14:20 material.config
-rw-r--r--. 1 sandbox users    2311 Jun 24 14:22 mesh_40grains.vtr
-rw-r--r--. 1 sandbox users    1751 Jun 24 14:22 seeds_40grains.vtu
```

Copy here in this directory (i.e., PK02)

Copy (cp) this file from location PK01 which is in one level up directory (../PK01)

```
[sandbox@materials25 PK02]$ cp ../PK01/tensionY.load .
[sandbox@materials25 PK02]$ ll
total 2188
-rw-r--r--. 1 sandbox users   12638 Jun 24 14:19 40grains.geom
-rw-r--r--. 1 sandbox users 1100085 Jun 24 14:22 40grains_tensionY_ipbased.vtk
-rw-r--r--. 1 sandbox users 1100088 Jun 24 14:22 40grains_tensionY_nodebased.vtk
-rw-r--r--. 1 sandbox users    6446 Jun 24 14:20 material.config
-rw-r--r--. 1 sandbox users    2311 Jun 24 14:22 mesh_40grains.vtr
-rw-r--r--. 1 sandbox users    1751 Jun 24 14:22 seeds_40grains.vtu
-rw-r--r--. 1 sandbox users      76 Jun 25 18:18 tensionY.load
```

```
[sandbox@materials25 PK02]$ nano material.config
```

sandbox@materials25:~/praveenk/PK02

```
  GNU nano 2.0.9                File: material.config

$Id: geom_fromVoronoiTessellation.py 4232M 2015-06-17 02:52:24Z (local) $ --config 40grains.seeds

<homogenization>
[SX]
type none

<crystallite>
[essential]
(output) texture
(output) f
(output) p
(output) orientation
(output) grainrotation

<phase>
{/opt/DAMASK/code/config/Phase_J2_AluminumIsotropic.config}

<microstructure>

                              [ Read 300 lines ]
^G Get Help    ^O WriteOut    ^R Read File    ^Y Prev Page    ^K Cut Text    ^C Cur Pos
^X Exit        ^J Justify     ^W Where Is     ^V Next Page    ^U UnCut Text  ^T To Spell
```

Editing "material.config" file to change the materials model from "isotropic" to "Phenomenological power law"

```
<phase>
{/opt/DAMASK/code/config/Phase_Phenopowerlaw_Aluminum.config}

<microstructure>


^G Get Help    ^O WriteOut    ^R Read File    ^Y Prev Page    ^K Cut Text    ^C Cur Pos
^X Exit        ^J Justify     ^W Where Is     ^V Next Page    ^U UnCut Text  ^T To Spell
```

sandbox@materials25:/opt/DAMASK/code/config

```
### $Id: Phase_Phenopowerlaw_Aluminum.config 4140 2015-05-05 20:17:50Z MPIE\m.diehl $ ###
[Aluminum]
elasticity              hooke
plasticity              phenopowerlaw

(output)                resistance_slip
(output)                shearrate_slip
(output)                resolvedstress_slip
(output)                accumulated_shear_slip
(output)                totalshear
(output)                resistance_twin
(output)                shearrate_twin
(output)                resolvedstress_twin
(output)                accumulated_shear_twin
(output)                totalvolfrac_twin

lattice_structure       fcc
Nslip                   12                  # per family
Ntwin                    0                  # per family

c11                     106.75e9
c12                     60.41e9
c44                     28.34e9

gdot0_slip      ?       0.001
n_slip          ?       20
tau0_slip       ?         31e6              # per family
tausat_slip     ?         63e6              # per family
a_slip          ?       2.25
gdot0_twin      ?       0.001
n_twin          ?       20
tau0_twin       ?         31e6              # per family
s_pr            ?       0                   # push-up factor for slip saturation due to twinning
twin_b          ?       0
twin_c          ?       0
twin_d          ?       0
twin_e          ?       0
h0_slipslip     ?       75e6
h0_twinslip             0
Phase_Phenopowerlaw_Aluminum.config
```

Hookean elasticity

Phenomenological power law (check next slide for details)

Output – resistance to slip along a slip system, shear rate, resolve shear stress along a slip system, total shear strain on a slip system, total shear in material, and similar terms for twin

Crystal structure

Number of primary slip systems

Number of twin systems (assumed 0 – i.e., no twinning allowed)

Stiffness tensor: C11, C22 and C44 (cubic)

tau0 – shear stress for slip on one plane, tausat – saturation stress, atol_resistance is a convergence parameter, and for other terms here, refer to next page (note w0 = a)

```
h0_twinslip             0
h0_twintwin             0
interaction_slipslip    1 1 1.4 1.4 1.4 1.4
interaction_sliptwin    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
interaction_twinslip    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
interaction_twintwin    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
atol_resistance         1
(END)
```

Relative intensity of 6 types of dislocation – dislocation interactions in this sequence: collinear, Lomer-Cottrell…????

```
[sandbox@materials25 PK02]$ DAMASK_spectral --load tensionY.load --geom 40grains.geom >40grains_tensionY.out &
[1] 13054
[sandbox@materials25 PK02]$
```

Job number at "server" computer

Run simulation (DAMASK software, Spectral method)

Using these load and geometry

Write solution in this file

Run in background

sandbox@materials25:~/praveenk/PK02

```
[sandbox@materials25 PK02]$ DAMASK_spectral --load tensionY.load --geom 40grains.geom >40grains_tensionY.out &
[1] 13054
[sandbox@materials25 PK02]$ ll
total 8144
-rw-r--r--. 1 sandbox users   12638 Jun 24 14:19 40grains.geom
-rw-r--r--. 1 sandbox users     648 Jun 25 18:53 40grains_tensionY.C_ref
-rw-r--r--. 1 sandbox users 1100085 Jun 25 18:53 40grains_tensionY_ipbased.vtk
-rw-r--r--. 1 sandbox users 1005058 Jun 25 18:53 40grains_tensionY.mesh
-rw-r--r--. 1 sandbox users 1100088 Jun 25 18:53 40grains_tensionY_nodebased.vtk
-rw-r--r--. 1 sandbox users 2409201 Jun 25 18:55 40grains_tensionY.out
-rw-r--r--. 1 sandbox users     267 Jun 25 18:53 40grains_tensionY.outputConstitutive
-rw-r--r--. 1 sandbox users      77 Jun 25 18:53 40grains_tensionY.outputCrystallite
-rw-r--r--. 1 sandbox users     148 Jun 25 18:53 40grains_tensionY.outputHomogenization
-rw-r--r--. 1 sandbox users 2654565 Jun 25 18:53 40grains_tensionY.spectralOut
-rw-r--r--. 1 sandbox users     185 Jun 25 18:54 40grains_tensionY.sta
-rw-r--r--. 1 sandbox users    6448 Jun 25 18:26 material.config
-rw-r--r--. 1 sandbox users    2311 Jun 24 14:22 mesh_40grains.vtr
-rw-r--r--. 1 sandbox users    1751 Jun 24 14:22 seeds_40grains.vtu
-rw-r--r--. 1 sandbox users      76 Jun 25 18:18 tensionY.load
[sandbox@materials25 PK02]$
```

Also important files

"tail" 40grains_tensionY.out to check the progress

```
[sandbox@materials25 PK01]$ tail -f 40grains_tensionY.out
```

sandbox@materials25:~/praveenk/PK02

```
... doing gamma convolution ...............................................

... evaluating constitutive response ......................................

Piola-Kirchhoff stress / MPa =
      0.0153         3.1500        -0.6039
      3.1799        85.9265        -0.5813
     -0.6066        -0.5785        34.4577

... calculating divergence ................................................

... doing gamma convolution ...............................................

... reporting .............................................................

error divergence =          2.09 (8.98E+04 / m, tol = 4.30E+04)
error stress BC =           0.02 (1.53E+04 Pa,  tol = 8.59E+05)

------------------------------------------------------------------------
Increment 10/200-1/1 @ Iteration 001≤003≤250

deformation gradient aim =
  0.955508     0.0000000     0.0000000
  0.000000     1.0050000     0.0000000
  0.000000     0.0000000     1.0000000

... evaluating constitutive response ......................................

Piola-Kirchhoff stress / MPa =
     -0.0017         3.1499        -0.6045
      3.1798        85.9150        -0.5820
     -0.6072        -0.5791        34.4474

... calculating divergence ................................................

... doing gamma convolution ...............................................

... evaluating constitutive response .......................................
```

10th out of 200 steps

Next iteration value for the stress tensor – it may take a few more steps

```
 increment 200 converged
STOP 0

 ... writing results to file ...............................

 ============================================================================
 000200 out of 000200 (100.0 %) increments converged!

DAMASK terminated on:
Date:                25/06/2015
Time:                19:23:24
```

Simulation run finishes

"Ctrl + C" to finish "tail"

```
[sandbox@materials25 PK02]$ less 40grains_tensionY.sta
Increment Time CutbackLevel Converged IterationsNeeded
          1  0.50000000000000000                0 T                3
          2   1.0000000000000000                0 T                7
          3   1.5000000000000000                0 T               12
          4   2.0000000000000000                0 T               10
          5   2.5000000000000000                0 T                9
          6   3.0000000000000000                0 T                8
          7   3.5000000000000000                0 T                7
          8   4.0000000000000000                0 T                6
          9   4.5000000000000000                0 T                6
         10   5.0000000000000000                0 T                5
         11   5.5000000000000000                0 T                5
         12   6.0000000000000000                0 T                4
         13   6.5000000000000000                0 T                4
         14   7.0000000000000000                0 T                4
         15   7.5000000000000000                0 T                4
         16   8.0000000000000000                0 T                3
         17   8.5000000000000000                0 T                4
         18   9.0000000000000000                0 T                3
         19   9.5000000000000000                0 T                4
         20   10.000000000000000                0 T                3
         21   10.500000000000000                0 T                3
         22   11.000000000000000                0 T                3
         23   11.500000000000000                0 T                3
         24   12.000000000000000                0 T                3
         25   12.500000000000000                0 T                3
         26   13.000000000000000                0 T                3
         27   13.500000000000000                0 T                3
         28   14.000000000000000                0 T                3
         29   14.500000000000000                0 T                3
         30   15.000000000000000                0 T                3
         31   15.500000000000000                0 T                3
         32   16.000000000000000                0 T                3
         33   16.500000000000000                0 T                3
         34   17.000000000000000                0 T                3
         35   17.500000000000000                0 T                3
         36   18.000000000000000                0 T                3
         37   18.500000000000000                0 T                3
         38   19.000000000000000                0 T                3
```

```
        194   97.000000000000000                0 T                3
        195   97.500000000000000                0 T                2
        196   98.000000000000000                0 T                3
        197   98.500000000000000                0 T                3
        198   99.000000000000000                0 T                2
        199   99.500000000000000                0 T                3
        200   100.00000000000000                0 T                3
(END)
```

"less" 40grains_tensionY.sta

Check for an increase and then a decrease and then finally a stable number of iterations to converge to a solution

- Now, either we can “postProc” data at increment step (as we did in the last example) or write the following shell program using “nano” with list of commands in same sequence as earlier, save it with some name (such as do_postprocess.sh), and run all it in one go!

```
#!/bin/bash

postResults 40grains_tensionY.spectralOut \
 --increments \
 --range 0 200 40 \
 --separation x,y,z \
 --split \
 --cr texture,f,p,orientation,grainrotation

cd postProc

theFile=40grains_tensionY_inc

addStrainTensors ${theFile}???.txt --left --logarithmic
addCauchy        ${theFile}???.txt
addMises         ${theFile}???.txt --strain 'ln(V)' --stress Cauchy
addIPFcolor      ${theFile}???.txt --pole 0 0 1 --symmetry cubic --quaternion orientation

imageData        ${theFile}???.txt \
  --label 'Mises(ln(V))' \
  --range 0 0.3 \
  --dimension 64 64 \
  --color green --invert

imageData        ${theFile}???.txt \
  --label 'Mises(Cauchy)' \
  --range 0 150e6 \
  --dimension 64 64 \
  --color red --invert

imageData        ${theFile}???.txt \
  --label '4_grainrotation' \
  --range 0 20 \
  --dimension 64 64

imageDataRGB     ${theFile}???.txt \
  --label IPF_001_cubic \
  --dimension 64 64
do_postprocess.sh (END)
```

Creates a folder postProc with results in a text file

Results from this file

Range up to 200 in increment of 40 (data: 0,40, 80, 120, 160 and 200)

New line (otherwise the whole sequence of command has to be written in one line without “line break”

These results

*After this step, we have 5 text files (*_inc40.txt, *_inc80.txt, etc.) in postProc folder with results at increments of 40*

Go inside postProc folder where files are created

String variable “theFile”

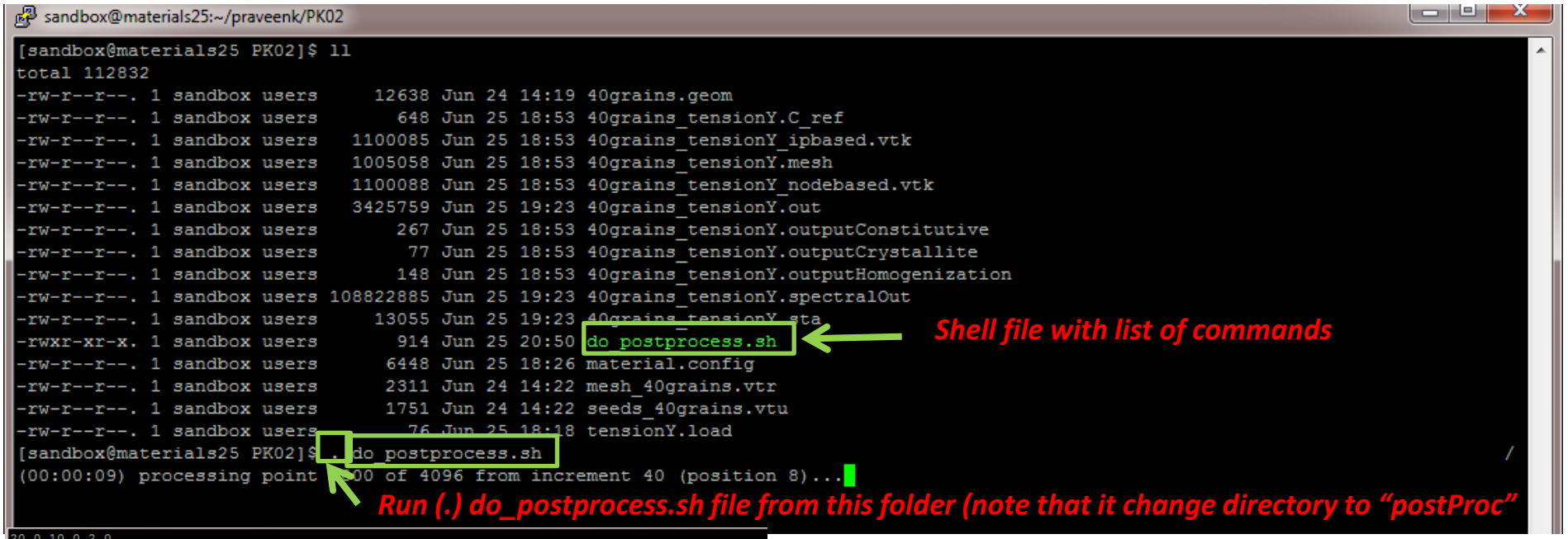
Add strain tensors, Cauchy stress, Mises strain and IPF information in the text file (name theFilexx – xxx is increment like 040, 080,…,200) using usual calculations

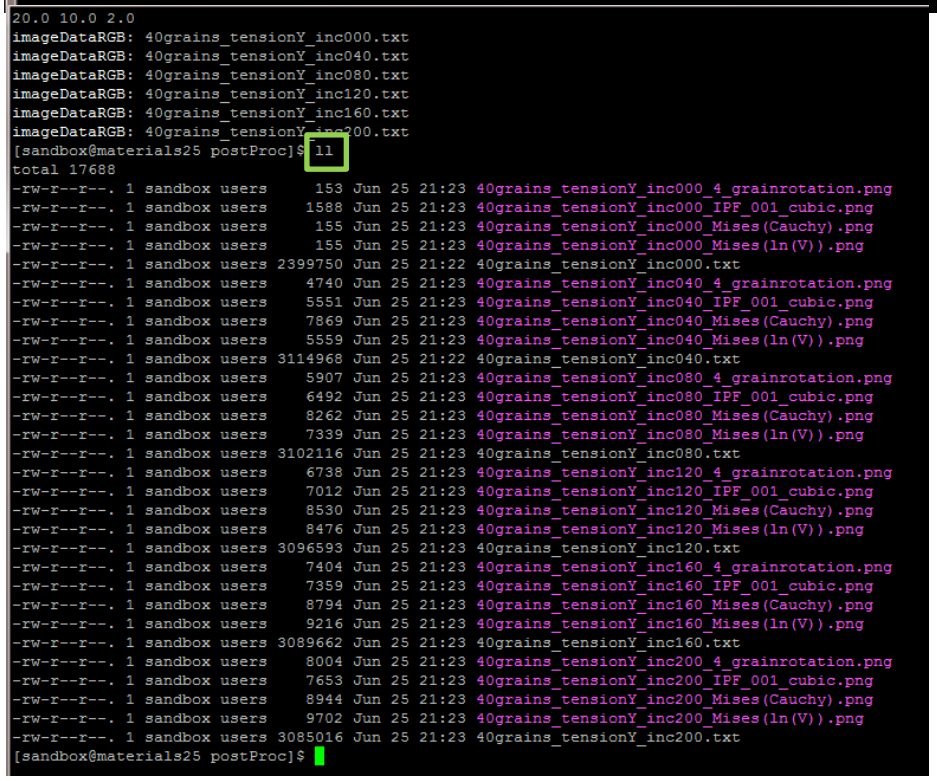
Generate image with 64 x 64 pixels showing Mises strain within range from 0 to 0.3 in green colour (invert ??) – File name: 40grains_tensionY_incxxx_Mises(ln(V)).png

Generate “red” image showing Cauchy stress File name: 40grains_tensionY_incxxx_Cauchy.png

Generate “greyscale” image showing Grain rotation File name: 40grains_tensionY_incxxx_grainrotation.png

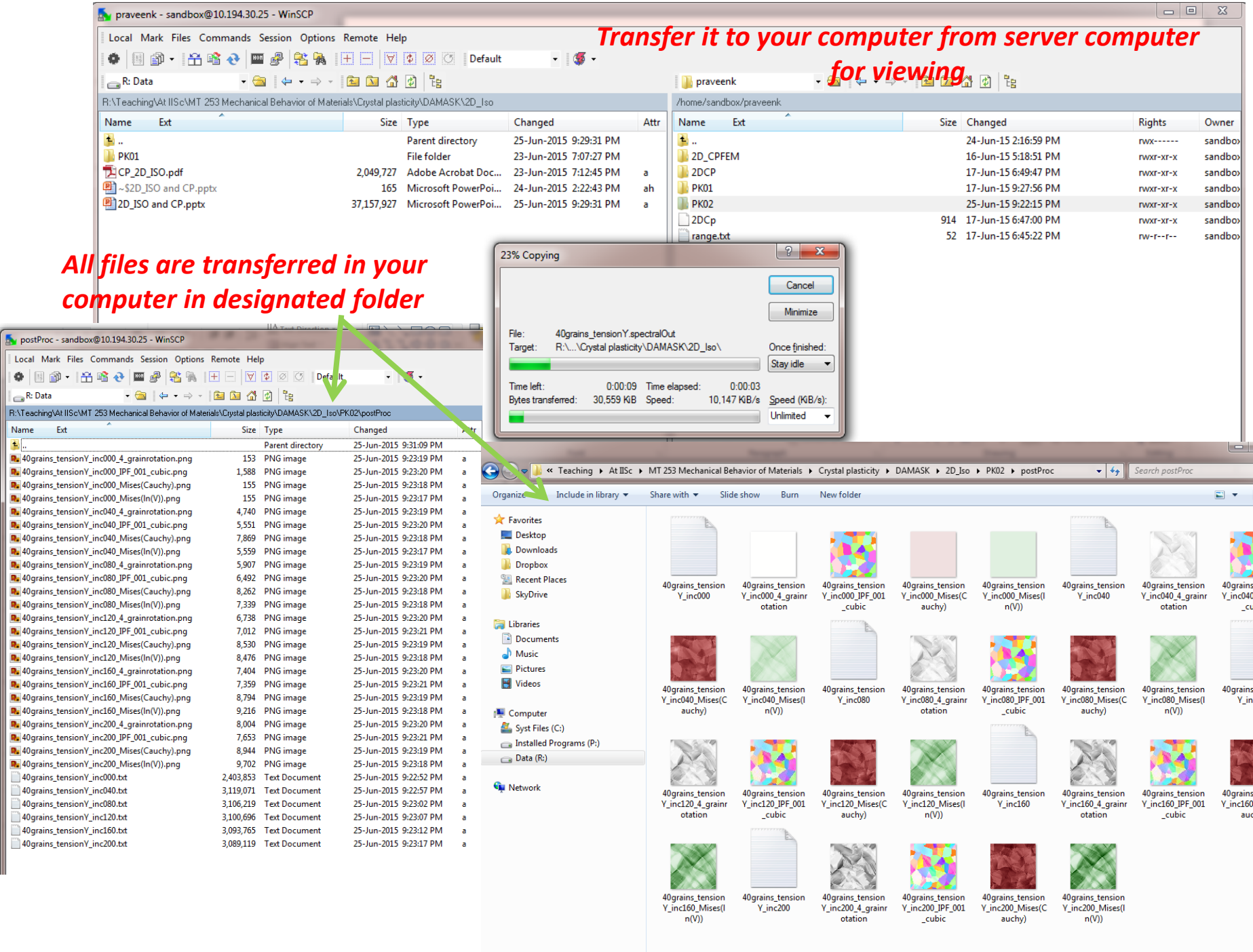
Generate RGB image showing IPF maps File name: 40grains_tensionY_incxxx_IPF_001_cubic.png

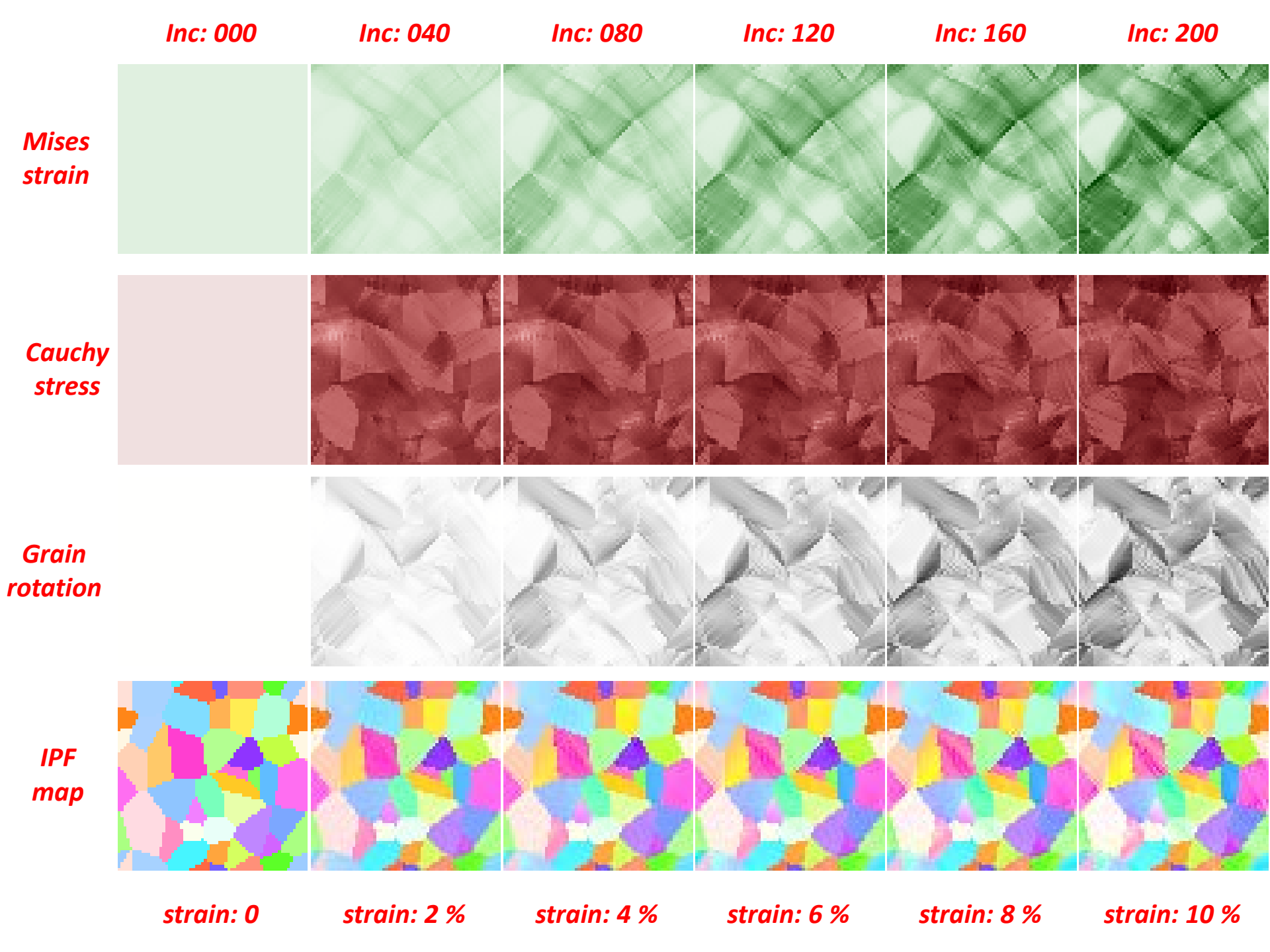




Check all text files (notice there names) and corresponding stress, strain, etc. files.

(One can do the same one by one also – or just go in one go ☺)

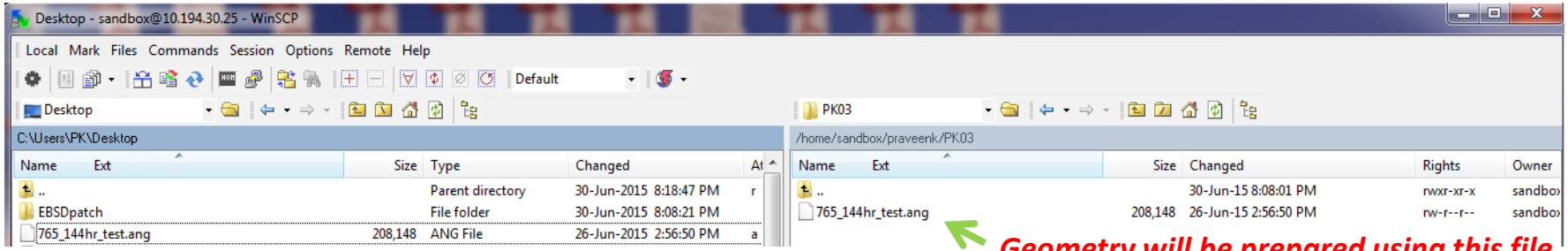

praveenk - sandbox@10.194.30.25 - WinSCP
Local Mark Files Commands Session Options Remote Help
R:\Teaching\At IISc\MT 253 Mechanical Behavior of Materials\Crystal plasticity\DAMASK\2D_Iso
/home/sandbox/praveenk
Transfer it to your computer from server computer for viewing
All files are transferred in your computer in designated folder
23% Copying
Cancel
Minimize
File: 40grains_tensionY.spectralOut
Target: R:\...\Crystal plasticity\DAMASK\2D_Iso\
Once finished:
Stay idle
Time left: 0:00:09
Time elapsed: 0:00:03
Bytes transferred: 30,559 KiB
Speed: 10,147 KiB/s
Speed (KiB/s):
Unlimited
postProc - sandbox@10.194.30.25 - WinSCP
R:\Teaching\At IISc\MT 253 Mechanical Behavior of Materials\Crystal plasticity\DAMASK\2D_Iso\PK02\postProc
Teaching ▸ At IISc ▸ MT 253 Mechanical Behavior of Materials ▸ Crystal plasticity ▸ DAMASK ▸ 2D_Iso ▸ PK02 ▸ postProc
Search postProc
Organize
Include in library
Share with
Slide show
Burn
New folder
Favorites
Desktop
Downloads
Dropbox
Recent Places
SkyDrive
Libraries
Documents
Music
Pictures
Videos
Computer
Syst Files (C:)
Installed Programs (P:)
Data (R:)
Network


Inc: 000
Inc: 040
Inc: 080
Inc: 120
Inc: 160
Inc: 200
Mises strain
Cauchy stress
Grain rotation
IPF map
strain: 0
strain: 2 %
strain: 4 %
strain: 6 %
strain: 8 %
strain: 10 %

Tutorial 3: Uniaxial compression type loading on a 2-phase alloy

```
[sandbox@materials25 praveenk]$ mkdir PK03
[sandbox@materials25 praveenk]$ ll
total 28
-rwxr-xr-x. 1 sandbox users  914 Jun 17 18:47 2DCp
drwxr-xr-x. 3 sandbox users 4096 Jun 17 18:49 2DCP
drwxr-xr-x. 3 sandbox users 4096 Jun 16 17:18 2D_CPFEM
drwxr-xr-x. 3 sandbox users 4096 Jun 17 21:27 PK01
drwxr-xr-x. 3 sandbox users 4096 Jun 25 21:22 PK02
drwxr-xr-x. 2 sandbox users 4096 Jun 30 20:08 PK03
-rw-r--r--. 1 sandbox users   52 Jun 17 18:45 range.txt
[sandbox@materials25 praveenk]$ cd PK03
[sandbox@materials25 PK03]$ pwd
/home/sandbox/praveenk/PK03
[sandbox@materials25 PK03]$
```

Copy the appropriate ".ang" file to the current directory (EBSD data can be exported to .ang file using TSL-OIM software) – one can use WinSCP as usual



Geometry will be prepared using this file

```
/home/sandbox/praveenk/PK03
[sandbox@materials25 PK03]$ ll
total 0
[sandbox@materials25 PK03]$ ll
total 204
-rw-r--r--. 1 sandbox users 208148 Jun 26 14:56 765_144hr_test.ang
[sandbox@materials25 PK03]$
```

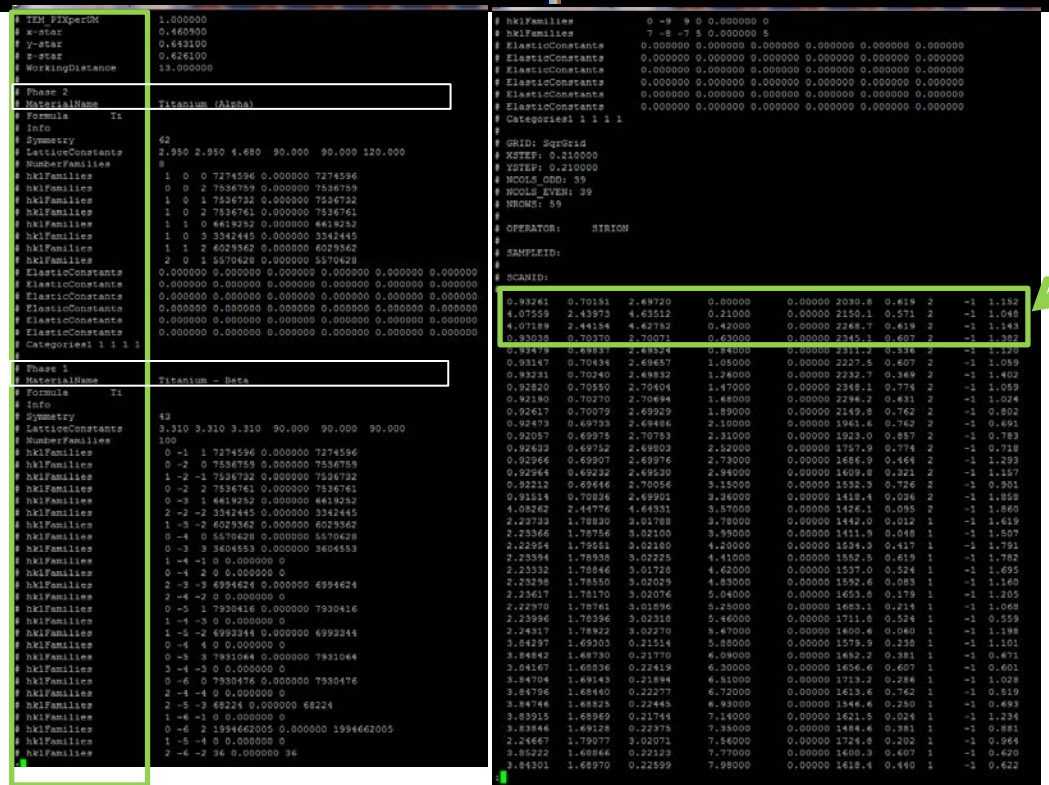
Steps for creating geometry file from .ang file

1. *Create .txt file from .ang by copying it in .txt format*
2. *Modify .txt file to add appropriate headers*
3. *Create geometry from table in the modified .txt file*

```
[sandbox@materials25 PK03]$ cp 765 144hr test.ang 765 144hr test.txt
[sandbox@materials25 PK03]$ ll
total 408
-rw-r--r--. 1 sandbox users 208148 Jun 26 14:56 765_144hr_test.ang
-rw-r--r--. 1 sandbox users 208148 Jun 30 20:23 765_144hr_test.txt
[sandbox@materials25 PK03]$
```

Create .txt file from .ang by copying it in .txt format

```
[sandbox@materials25 PK03]$ less 765 144hr_test.txt
```



Commented details of entries

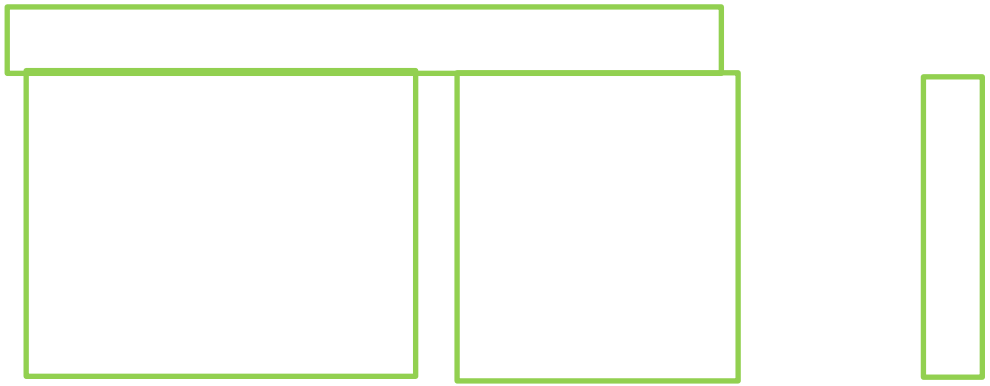
Table of data in following sequence:
Euler angles 1, 2 and 3, followed by x and y coordinates of the point, followed by some "useless (incomprehensible) information" followed by phase information
(1 and 2 are beta-Ti and alpha-Ti, respectively – as it comes from EBSD data itself!) followed by more useless information

```
[sandbox@materials25 PK03]$ nano 765 144hr test.txt
```

sandbox@materials25:~/praveenk/PK03

```
  GNU nano 2.0.9            File: 765_144hr_test.txt

# TEM_PIXperUM           1.000000
# x-star                 0.460900
# y-star                 0.643100
# z-star                 0.626100
# WorkingDistance        13.000000
#
# Phase 2
# MaterialName           Titanium (Alpha)
# Formula       Ti
# Info
# Symmetry               62
# LatticeConstants       2.950 2.950 4.680  90.000  90.000 120.000
# NumberFamilies         8
# hklFamilies             1   0   0 7274596 0.000000 7274596
# hklFamilies             0   0   2 7536759 0.000000 7536759
# hklFamilies             1   0   1 7536732 0.000000 7536732
# hklFamilies             1   0   2 7536761 0.000000 7536761
# hklFamilies             1   1   0 6619252 0.000000 6619252
# hklFamilies             1   0   3 3342445 0.000000 3342445
                [ Read 2419 lines (Converted from DOS format) ]
^G Get Help  ^O WriteOut  ^R Read File ^Y Prev Page ^K Cut Text  ^C Cur Pos
^X Exit      ^J Justify   ^W Where Is  ^V Next Page ^U UnCut Text^T To Spell
```

Delete all these (comment information) to convert the .txt file containing a clean table with Euler angles, coordinates, etc. with certain headers (^K or cut command may expedite deleting lines)



a,b, c and d are useless information

```
[sandbox@materials25 PK03]$ showTable -l 765_144hr_test.txt

REMARK: h5py module not available

showTable: 765_144hr_test.txt
1_euler 2_euler 3_euler 1_pos   2_pos   a       b       phase   c       d
[sandbox@materials25 PK03]$
```

Show the labels (-l) of table in the .txt file

```
[sandbox@materials25 PK03]$ showTable -h

REMARK: h5py module not available

Usage: showTable [options] [file[s]]

 Show components of given ASCIItable(s).

Options:
  --version      show program's version number and exit
  -h, --help     show this help message and exit
  -a, --head     output all heading (info + labels)
  -i, --info     output info lines
  -l, --labels   output labels
  -d, --data     output data
  -c, --column   switch to label column format
  --nolabels     table has no labels
```

Get help (-h) with the extensions (i.e., things after "-")

So "showTable –d will show data in the table

```
[sandbox@materials25 PK03]$ showTable -d 765_144hr_test.txt | wc -l

REMARK: h5py module not available

showTable: 765_144hr_test.txt
2262
```

Count (wc) the lines (-l) of data in the table (-d)

Only 58 x 39 (that's the number of grid points – note it was 64 x 64 in previous two examples) → anyway, there are 59 x 39 in EBSD data, somehow one row is lost here!

```
[sandbox@materials25 PK03]$ showTable -d 765_144hr_test.txt
```

Show the table data (use "showTable –d filename.txt | less" command at the end to read data page by page

```
2.24851 1.80418 3.02589 0.84000 8.61000 1702.1  0.464   1       -1      0.747
5.85292 2.87956 3.59045 1.05000 8.61000 1680.1  0.679   1       -1      0.675
5.81768 2.88301 3.55636 1.26000 8.61000 1750.3  0.536   1       -1      0.620
2.24202 1.80470 3.02473 1.47000 8.61000 1821.3  0.476   1       -1      0.497
2.24199 1.79947 3.02413 1.68000 8.61000 1852.8  0.500   1       -1      0.419
5.86606 2.87880 3.60756 1.89000 8.61000 1819.6  0.595   1       -1      0.859
2.24652 1.80399 3.03163 2.10000 8.61000 1766.0  0.286   1       -1      0.823
1.44154 1.65613 4.55592 2.31000 8.61000 2187.5  0.774   2       -1      0.572
4.58092 1.48477 4.86600 2.52000 8.61000 2803.0  0.798   2       -1      0.539
4.57902 1.48557 4.86718 2.73000 8.61000 2806.9  0.821   2       -1      0.531
4.57726 1.48255 4.86658 2.94000 8.61000 2938.2  0.702   2       -1      0.640
4.57963 1.48561 4.86387 3.15000 8.61000 2809.7  0.798   2       -1      0.499
4.57616 1.48358 4.86514 3.36000 8.61000 2545.9  0.798   2       -1      0.542
5.84259 2.87297 3.60220 3.57000 8.61000 1738.9  0.286   1       -1      1.102
5.84526 2.86388 3.60698 3.78000 8.61000 1815.4  0.512   1       -1      0.491
2.21851 1.81979 3.01501 3.99000 8.61000 1843.1  0.488   1       -1      0.792
2.21838 1.81891 3.01437 4.20000 8.61000 1960.5  0.179   1       -1      1.045
2.22323 1.81611 3.02024 4.41000 8.61000 1649.4  0.429   1       -1      0.866
2.22404 1.81755 3.02087 4.62000 8.61000 1622.5  0.262   1       -1      1.153
2.22884 1.81425 3.01968 4.83000 8.61000 1726.0  0.726   1       -1      0.745
2.23036 1.81451 3.02418 5.04000 8.61000 1706.0  0.286   1       -1      0.956
5.85278 2.86666 3.60207 5.25000 8.61000 1518.9  0.107   1       -1      0.913
5.85700 2.86290 3.61401 5.46000 8.61000 1531.7  0.262   1       -1      1.163
5.84653 2.86950 3.60854 5.67000 8.61000 1489.3  0.333   1       -1      0.969
0.69275 1.44745 1.32796 5.88000 8.61000 1429.9  0.357   1       -1      0.833
3.83588 1.69445 0.24357 6.09000 8.61000 1445.6  0.119   1       -1      1.103
2.24490 1.80362 3.01945 6.30000 8.61000 1439.7  0.202   1       -1      1.121
2.23523 1.81056 3.01832 6.51000 8.61000 1591.9  0.274   1       -1      0.707
3.83879 1.69215 0.23856 6.72000 8.61000 1620.3  0.524   1       -1      0.486
3.83564 1.69389 0.23898 6.93000 8.61000 1638.0  0.298   1       -1      0.907
2.23148 1.80624 3.01708 7.14000 8.61000 1565.0  0.548   1       -1      1.048
```

```
[sandbox@materials25 PK03]$ filterTable -h

REMARK: h5py module not available

Usage: filterTable options [file[s]]

 Filter rows according to condition and columns by either white or black
listing.  Examples: Every odd row if x coordinate is positive -- " #ip.x# >=
0.0 and #_row_#%2 == 1 ). All rows where label 'foo' equals 'bar' -- " #foo#
== "bar" "

Options:
  --version             show program's version number and exit
  -h, --help            show this help message and exit
  -w <string LIST>, --white=<string LIST>
                        white list of column labels (a,b,c,...)
  -b <string LIST>, --black=<string LIST>
                        black list of column labels (a,b,c,...)
  -c string, --condition=string
                        condition to filter rows
```

Get help (-h or --help) with the extensions (i.e., things after "-")

????

```
[sandbox@materials25 PK03]$ showTable -l 765_144hr_test.txt

REMARK: h5py module not available

showTable: 765_144hr_test.txt
1_euler 2_euler 3_euler 1_pos   2_pos   a       b       phase   c       d
[sandbox@materials25 PK03]$ filterTable < 765_144hr_test.txt -w '?_euler' -c '#_row_# == 1'

REMARK: h5py module not available

filterTable
2       header
$Id: filterTable.py 4217 2015-05-28 22:31:32Z p.eisenlohr $     -w ?_euler -c #_row_# == 1
1_euler 2_euler 3_euler
0.93261 0.70151 2.69720
```

Filter all Euler angles (?_euler) data from the first row of the table (#_row_# == 1)

--? – what is the use of this step?

First row data of Euler angles

```
[sandbox@materials25 PK03]$ geom_fromTable --help

REMARK: h5py module not available

Usage: geom_fromTable options [file[s]]

 Generate geometry description and material configuration from position,
phase, and orientation data.

Options:
  --version             show program's version number and exit
  -h, --help            show this help message and exit
  --coordinates=string  coordinates label
  --phase=string        phase label
  -e string, --eulers=string
                        Euler angles label
  -d, --degrees         angles are given in degrees [False]
  -m string, --matrix=string
                        orientation matrix label
  -a string             crystal frame a vector label
  -b string             crystal frame b vector label
  -c string             crystal frame c vector label
  -q string, --quaternion=string
                        quaternion label
  --axes=string string string
                        orientation coordinate frame in terms of position
                        coordinate frame [same]
  -s <string LIST>, --symmetry=<string LIST>
                        crystal symmetry [cubic] {orthorhombic, tetragonal,
                        hexagonal, cubic}
  -t float, --tolerance=float
                        angular tolerance for orientation squashing [0.0]
  --homogenization=int  homogenization index to be used [1]
  --crystallite=int     crystallite index to be used [1]
[sandbox@materials25 PK03]$
```

Get help (-h or --help) with the extensions (i.e., things after "-")

*Coordinates are under "*_pos", phase is under phase and eulers is under "*_euler" headings*

Orientation of x, y and z of geometru with that in "EBSD" file

List of symmetries

Tolerance in angle (radians)

```
[sandbox@materials25 PK03]$ geom_fromTable --coordinates pos --eulers euler --phase phase --axes -y -x -z -
-symmetry cubic,hexagonal 765_144hr_test.txt --tolerance 0.02

REMARK: h5py module not available

geom_fromTable: 765_144hr_test.txt
.....
grid     a b c: 39 x 58 x 1
size     x y z: 7.98 x 11.97 x 0.204615384615
origin   x y z: 0.0 : 0.0 : 0.0
homogenization: 1
microstructures: 91
[sandbox@materials25 PK03]$
```

Creating geometry file from table data in .txt file while specifying coordinates, Euler angles, phases, axes relationship between geometry and the original EBSD/.ang file, crystal symmetries and the tolerance in angle (Note: the sequence of "--" commands so not matter!)

No homogenization scheme as each point is defined as a crystallite

Only 91 grains

```
[sandbox@materials25 PK03]$ ll
total 428
-rw-r--r--. 1 sandbox users 208148 Jun 26 14:56 765_144hr_test.ang
-rw-r--r--. 1 sandbox users  22221 Jun 30 21:44 765_144hr_test.geom
-rw-r--r--. 1 sandbox users 201377 Jun 30 20:53 765_144hr_test.txt
[sandbox@materials25 PK03]$ less 765_144hr_test.geom
```

```
554     header
$Id: geom_fromTable.py 4279 2015-06-21 11:56:05Z p.eisenlohr $ --coordinates pos --eulers euler --phase pha
se --axes -y -x -z --symmetry cubic,hexagonal 765_144hr_test.txt --tolerance 0.02
grid    a 39    b 58    c 1
size    x 7.980000      y 11.970000     z 0.204615
origin  x 0.000000      y 0.000000      z 0.000000
homogenization  1
microstructures 91
<microstructure>
[Grain01]
crystallite 1
(constituent)   phase 2 texture  1      fraction 1.0
[Grain02]
crystallite 1
(constituent)   phase 1 texture  2      fraction 1.0
[Grain03]
crystallite 1
(constituent)   phase 1 texture  3      fraction 1.0
[Grain04]
crystallite 1
(constituent)   phase 2 texture  4      fraction 1.0
[Grain05]
crystallite 1
(constituent)   phase 1 texture  5      fraction 1.0
[Grain06]
crystallite 1
(constituent)   phase 1 texture  6      fraction 1.0
[Grain07]
```

Creating a materials.config file from the .geom file itself (note – earlier we created material.config file using Voronoi Tessellation on the seed points; however, we do not need any tessellation here as geom file already has all information about grain definition, etc.).

```
[sandbox@materials25 PK03]$ showTable --help

REMARK: h5py module not available

Usage: showTable [options] [file[s]]

 Show components of given ASCIItable(s).

Options:
  --version      show program's version number and exit
  -h, --help     show this help message and exit
  -a, --head     output all heading (info + labels)
  -i, --info     output info lines
  -l, --labels   output labels
  -d, --data     output data
  -c, --column   switch to label column format
  --nolabels     table has no labels
[sandbox@materials25 PK03]$
```

Output comes as rows ??

This does not include labels

```
[sandbox@materials25 PK03]$ showTable --nolabel --info 765_144hr_test.geom | tail -n 548 > material.config

REMARK: h5py module not available

showTable: 765_144hr_test.geom
[sandbox@materials25 PK03]$ ll
total 444
-rw-r--r--. 1 sandbox users 208148 Jun 26 14:56 765_144hr_test.ang
-rw-r--r--. 1 sandbox users  22221 Jun 30 21:44 765_144hr_test.geom
-rw-r--r--. 1 sandbox users 201377 Jun 30 20:53 765_144hr_test.txt
-rw-r--r--. 1 sandbox users  15101 Jun 30 22:58 material.config
```

Writes the bottom 548 (?) lines in material.config file

-- see the difference in .config and .geom file in next slide

```
sandbox@materials25:~/praveenk/PK03
[sandbox@materials25 PK03]$ less material.config
<microstructure>
[Grain01]
crystallite 1
(constituent)   phase 2 texture  1      fraction 1.0
[Grain02]
crystallite 1
(constituent)   phase 1 texture  2      fraction 1.0
[Grain03]
crystallite 1
(constituent)   phase 1 texture  3      fraction 1.0
[Grain04]
crystallite 1
(constituent)   phase 2 texture  4      fraction 1.0
[Grain05]
crystallite 1
(constituent)   phase 1 texture  5      fraction 1.0
[Grain06]
crystallite 1
(constituent)   phase 1 texture  6      fraction 1.0
[Grain07]
crystallite 1
(constituent)   phase 1 texture  7      fraction 1.0
[Grain08]
crystallite 1
(constituent)   phase 1 texture
[Grain09]
crystallite 1
(constituent)   phase 2 texture
[Grain10]
crystallite 1
(constituent)   phase 1 texture
[Grain11]
crystallite 1
(constituent)   phase 2 texture
[Grain12]
crystallite 1
```

Thus, other way of making "material.config" file is to copy .geom file to material.config file, open the material.config file (say using nano or even Notepad ++) and delete the top non-essential stuffs → this may be useful if it is difficult to calculate 548 number (??)

```
sandbox@materials25:~/praveenk/PK03
[sandbox@materials25 PK03]$ less 765_144hr_test.geom
$Id: geom_fromTable.py 4279 2015-06-21 11:56:05Z p.eisenlohr $ --coordinates pos --eulers euler --phase phase --axes -y -x -z --symmetry cubic,hexagonal 7
65_144hr_test.txt --tolerance 0.02
grid    a 39    b 58    c 1
size    x 7.980000      y 11.970000     z 0.204615
origin  x 0.000000      y 0.000000      z 0.000000
homogenization  1
microstructures 91
<microstructure>
[Grain01]
crystallite 1
(constituent)   phase 2 texture  1      fraction 1.0
[Grain02]
crystallite 1
(constituent)   phase 1 texture  2      fraction 1.0
[Grain03]
crystallite 1
(constituent)   phase 1 texture  3      fraction 1.0
[Grain04]
crystallite 1
(constituent)   phase 2 texture  4      fraction 1.0
[Grain05]
crystallite 1
(constituent)   phase 1 texture  5      fraction 1.0
[Grain06]
crystallite 1
(constituent)   phase 1 texture  6      fraction 1.0
[Grain07]
crystallite 1
(constituent)   phase 1 texture  7      fraction 1.0
[Grain08]
crystallite 1
(constituent)   phase 1 texture  8      fraction 1.0
[Grain09]
crystallite 1
(constituent)   phase 2 texture  9      fraction 1.0
```

All that is gone in .config file (as that is not in bottom 548 lines!)

Same

Editing material.config file to include options for homogenization, output and phases

```
[sandbox@materials25 PK03]$ nano material.config
```

sandbox@materials25:~/praveenk/PK03

```
 GNU nano 2.0.9                    File: material.config

<homogenization>
[none]
type none

<crystallite>
[aLittle]
(output) phase
(output) f
(output) p
(output) orientation
(output) grainrotation

<phase>
{/opt/DAMASK/code/config/Phase_Phenopowerlaw_BCC-Ferrite.config}

{/opt/DAMASK/code/config/Phase_Phenopowerlaw_cpTi-alpha.config}

<microstructure>
[Grain01]
crystallite 1
(constituent)   phase 2 texture  1      fraction 1.0
[Grain02]
crystallite 1
(constituent)   phase 1 texture  2      fraction 1.0
[Grain03]
crystallite 1
(constituent)   phase 1 texture  3      fraction 1.0
[Grain04]
crystallite 1
(constituent)   phase 2 texture  4      fraction 1.0
[Grain05]
crystallite 1

^G Get Help   ^O WriteOut   ^R Read File   ^Y Prev Page   ^K Cut Text   ^C Cur Pos
^X Exit       ^J Justify    ^W Where Is    ^V Next Page   ^U UnCut Text ^T To Spell
```

No homogenization

Crystal related outputs of phase information, displacement gradient, stress tensor, orientation and grain orientation will be generated / calculated

Two phase (first appearing is first phase)
→ BCC ferrite is used for beta-Ti (which is BCC) - phase 1
→ Cp-Ti is used for alpha-Ti (which is HCP) – phase 2

```
[sandbox@materials25 PK03]$ head material.config
<homogenization>
[none]
type none

<crystallite>
[aLittle]
(output) phase
(output) f
(output) p
(output) orientation
```

To read top 10 lines – as a cross-check of saving the changes in a file

Writing the load file (uniaxial compression at rate of 10^{-3} s^{-1})

```
[sandbox@materials25 PK03]$ nano compressionY.load
```

```
 GNU nano 2.0.9                File: compressionY.load                    Modified

Fdot * 0 0 0 -1e-3 0 0 0 0 stress 0 * * * * * * * * time 200 incs 100 freq 5

^G Get Help  ^O WriteOut  ^R Read File  ^Y Prev Page  ^K Cut Text  ^C Cur Pos
^X Exit      ^J Justify   ^W Where Is   ^V Next Page  ^U UnCut Text ^T To Spell
```

I

1. ** represents unconstrained BC*
2. *Strain rate in y direction is 10^{-3} s^{-1}*
3. *Stress in x-direction must be zero (traction free)*
4. *Load it for 200 seconds (i.e., up to 0.2 strain)*
5. *Total increments to finish is 100 (i.e. each time step is of 2 seconds)*
6. *Save data with frequency of 5 – so total 20 sets of data will be saved*

```
[sandbox@materials25 PK03]$ ls -rtl
total 448
-rw-r--r--. 1 sandbox users 208148 Jun 26 14:56 765_144hr_test.ang
-rw-r--r--. 1 sandbox users 201377 Jun 30 20:53 765_144hr_test.txt
-rw-r--r--. 1 sandbox users  22221 Jun 30 21:44 765_144hr_test.geom
-rw-r--r--. 1 sandbox users  15381 Jun 30 23:19 material.config
-rw-r--r--. 1 sandbox users     77 Jun 30 23:30 compressionY.load
```

Same as "ll" (long–list)

II

Running DAMASK Simulation on more than 1 node (☺)

```
sandbox@materials25:~/praveenk/PK03
[sandbox@materials25 PK03]$ cat /proc/cpuinfo | grep processor | wc -l
24
[sandbox@materials25 PK03]$ echo $DAMASK_NUM_THREADS
1
[sandbox@materials25 PK03]$ export DAMASK_NUM_THREADS=4
[sandbox@materials25 PK03]$ echo $DAMASK_NUM_THREADS
4
[sandbox@materials25 PK03]$
```

How many nodes are available

How many are used by DAMASK now

Run DAMASK on 4 nodes

```
[sandbox@materials25 PK03]$ DAMASK_spectral --load compressionY.load --geom 765_144hr_test.geom > 765_144hr_test_compressionY.out &
[1] 28023
[sandbox@materials25 PK03]$
```

Run simulation

Job number at "server" computer

Using these load and geometry

Write solution in this file

Run in background

```
[sandbox@materials25 PK03]$ tail -f 765_144hr_test_compressionY.out
```

Follow as the simulation runs (on 4 nodes, it will run very fast)

```
... evaluating constitutive response .....

Piola--Kirchhoff stress / MPa =
      0.0574       59.0264      -68.8214
     57.2595     -581.7319        8.8904
    -67.8477        9.0364     -186.7896

... calculating divergence .....

... doing gamma convolution .....

... evaluating constitutive response .....

Piola--Kirchhoff stress / MPa =
     -0.0353       59.0371      -68.8191
     57.2683     -581.6450        8.8637
    -67.8469        9.0088     -186.8648

... calculating divergence .....

... doing gamma convolution .....

... reporting .....

error divergence =         6.72 (1.95E+06 / m, tol = 2.91E+05)
error stress BC =          0.01 (3.53E+04 Pa,  tol = 5.82E+06)

================================================================
Increment 8/100-1/1 @ Iteration 001≤004≤250

deformation gradient aim =
  1.0143628    0.0000000    0.0000000
  0.0000000    0.9840000    0.0000000
  0.0000000    0.0000000    1.0000000

... evaluating constitutive response .....
```

```
... doing gamma convolution .....

... reporting .....

error divergence =      4183.10 (5.94E+09 / m, tol = 1.42E+06)
error stress BC =         60.17 (1.71E+09 Pa,  tol = 2.84E+07)

Increment 80/100-7/8 @ Iteration 001≤004≤250

deformation gradient aim =
  1.2927539    0.0000000    0.0000000
  0.0000000    0.8402500    0.0000000
  0.0000000    0.0000000    1.0000000

... evaluating constitutive response .....
Integration point          1  at element        2079  terminally ill
cc HOMOG >> Material Point terminally ill
```

```
+-------------------------------------------------------+
+                       warning                         +
+                         850                           +
+                                                       +
+ max number of cut back exceeded, terminating         +
+-------------------------------------------------------+
STOP 2

DAMASK terminated on:
Date:                30/06/2015
Time:                23:58:53
```

Cut back exceeded ??

```
--Kirchhoff stress / MPa =
 707.6618       7.8008     105.7889
-24.7688   -2838.0433      95.5862
 -8.5172      -2.9110   -2000.0037

alculating divergence .....

oing gamma convolution .....

valuating constitutive response .....

--Kirchhoff stress / MPa =
 707.6618       7.8008     105.7889
-24.7688   -2838.0433      95.5862
 -8.5172      -2.9110   -2000.0037

... calculating divergence .....

... doing gamma convolution .....
restart information available at      1

... reporting .....

error divergence =      4183.10 (5.94E+09 / m, tol = 1.42E+06)
error stress BC =         60.17 (1.71E+09 Pa,  tol = 2.84E+07)
```

Could not converge beyond 80 steps (i.e., slightly less than 16 % strain)

sandbox@materials25:~/praveenk/PK03

Increment	Time	CutbackLevel	Converged	IterationsNeeded
1	2.0000000000000000	0	T	9
2	4.0000000000000000	0	T	34
3	6.0000000000000000	0	T	15
4	8.0000000000000000	0	T	13
5	10.000000000000000	0	T	12
6	12.000000000000000	0	T	12
7	14.000000000000000	0	T	11
8	16.000000000000000	0	T	11
9	18.000000000000000	0	T	10
10	20.000000000000000	0	T	10
11	22.000000000000000	0	T	10
12	24.000000000000000	0	T	9
13	26.000000000000000	0	T	9
14	28.000000000000000	0	T	9
15	30.000000000000000	0	T	9
16	32.000000000000000	0	T	9
17	34.000000000000000	0	T	9
18	36.000000000000000	0	T	9
19	38.000000000000000	0	T	10
20	40.000000000000000	0	T	10
21	42.000000000000000	0	T	10
22	44.000000000000000	0	T	10
23	46.000000000000000	0	T	10
24	48.000000000000000	0	T	10
25	50.000000000000000	0	T	10
26	52.000000000000000	0	T	10
27	54.000000000000000	0	T	11
28	56.000000000000000	0	T	11
29	58.000000000000000	0	T	11
30	60.000000000000000	0	T	12
31	62.000000000000000	0	T	12
32	64.000000000000000	0	T	12
33	66.000000000000000	0	T	12
34	68.000000000000000	0	T	12
35	70.000000000000000	0	T	13
36	72.000000000000000	0	T	13
37	74.000000000000000	0	T	13
38	76.000000000000000	0	T	13
39	78.000000000000000	0	T	14
40	80.000000000000000	0	T	14
41	82.000000000000000	0	T	14
42	84.000000000000000	0	T	14
43	86.000000000000000	0	T	15
44	88.000000000000000	0	T	14
45	90.000000000000000	0	T	15
46	92.000000000000000	0	T	15
47	94.000000000000000	0	T	16
48	96.000000000000000	0	T	16

765_144hr_test_compressionY.sta

sandbox@materials25:~/praveenk/PK03

33	66.000000000000000	0	T	12
34	68.000000000000000	0	T	12
35	70.000000000000000	0	T	13
36	72.000000000000000	0	T	13
37	74.000000000000000	0	T	13
38	76.000000000000000	0	T	13
39	78.000000000000000	0	T	14
40	80.000000000000000	0	T	14
41	82.000000000000000	0	T	14
42	84.000000000000000	0	T	14
43	86.000000000000000	0	T	15
44	88.000000000000000	0	T	14
45	90.000000000000000	0	T	15
46	92.000000000000000	0	T	15
47	94.000000000000000	0	T	16
48	96.000000000000000	0	T	16
49	98.000000000000000	0	T	16
50	100.00000000000000	0	T	17
51	102.00000000000000	0	T	17
52	104.00000000000000	0	T	17
53	106.00000000000000	0	T	18
54	108.00000000000000	0	T	18
55	110.00000000000000	0	T	18
56	112.00000000000000	0	T	19
57	114.00000000000000	0	T	19
58	116.00000000000000	0	T	20
59	118.00000000000000	0	T	20
60	120.00000000000000	0	T	21
61	122.00000000000000	0	T	21
62	124.00000000000000	0	T	22
63	126.00000000000000	0	T	22
64	128.00000000000000	0	T	23
65	130.00000000000000	0	T	24
66	132.00000000000000	0	T	25
67	134.00000000000000	0	T	26
68	136.00000000000000	0	T	28
69	138.00000000000000	0	T	28
70	140.00000000000000	0	T	32
71	142.00000000000000	0	T	30
72	144.00000000000000	0	T	41
73	146.00000000000000	0	T	33
74	148.00000000000000	0	T	48
75	150.00000000000000	0	T	42
76	152.00000000000000	0	T	54
77	154.00000000000000	0	T	51
78	156.00000000000000	0	T	65
79	158.00000000000000	0	T	64
80	159.00000000000000	1	T	64
80	159.50000000000000	2	T	66

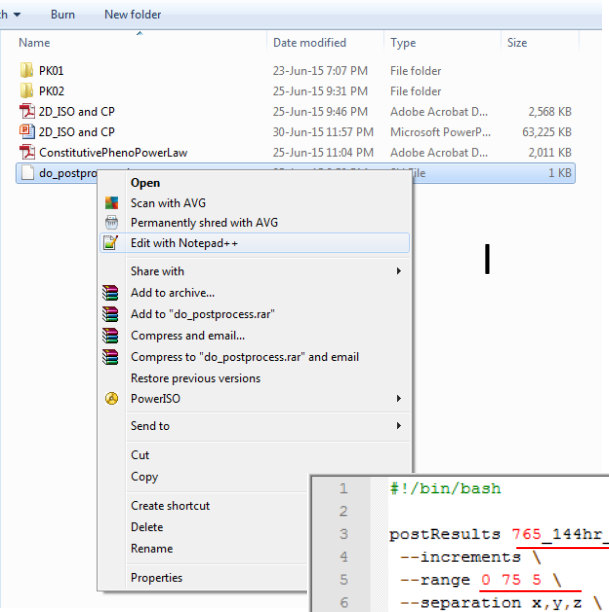
(END)

"less" the .sta file to check for steps required to converge to a solution

Check – it almost explodes at the end (most probably, a reduction in total strain or a increase in total increments (say 0.5 second per step instead of current 2 seconds per step) will help it converge???

We can use the same old shell program to do post processing for us – however, we need to modify it to suit this problem (look at range, only two question marks in file name (i.e., ?? Instead of ???), and assigning the proper name to IPF maps based on their phase number.

→ We can edit using "nano" in "putty" or text editor in "windows"



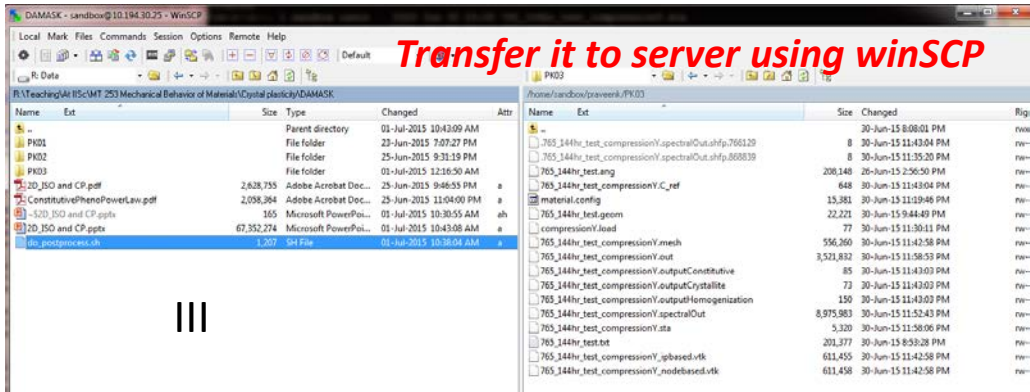
I

Windows – editing using Notepad ++

II

```
#!/bin/bash

postResults 765_144hr_test_compressionY.spectralOut \
 --increments \
 --range 0 75 5 \
 --separation x,y,z \
 --split \
 --cr phase,f,p,orientation,grainrotation

cd postProc

theFile=765_144hr_test_compressionY_inc

addStrainTensors ${theFile}??.txt --left --logarithmic
addCauchy        ${theFile}??.txt
addMises         ${theFile}??.txt --strain 'ln(V)' --stress Cauchy
addIPFcolor      ${theFile}??.txt --pole 0 0 1 --symmetry cubic --quaternion orientation
addIPFcolor      ${theFile}??.txt --pole 0 0 1 --symmetry hexagonal --quaternion orientation

for i in 1 2 3; do addCalculation -l "${i}_IPF_001" -f "#${i}_IPF_001_cubic# if #phase# == 1 else #${i}_IPF_001_hexagonal#" ${theFile}??.txt;done


imageData        ${theFile}??.txt \
  --label 'Mises(ln(V))' \
  --range 0 0.3 \
  --dimension 39 58 \
  --color green --invert

imageData        ${theFile}??.txt \
  --label 'Mises(Cauchy)' \
  --range 0 150e6 \
  --dimension 39 58 \
  --color red --invert

imageData        ${theFile}??.txt \
  --label '4_grainrotation' \
  --range 0 20 \
  --dimension 39 58

imageDataRGB     ${theFile}??.txt \
  --label IPF_001_cubic \
  --dimension 39 58
```

Transfer it to server using winSCP



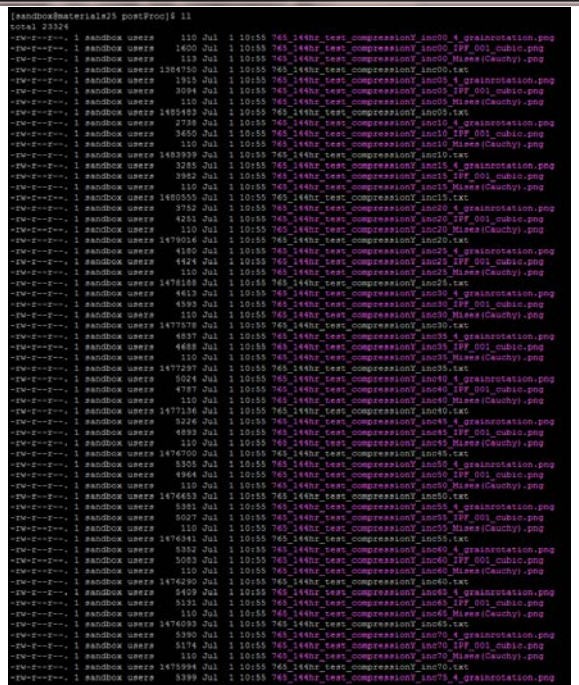
III

```
sandbox@materials25:~/praveenk/PK03
[sandbox@materials25 PK03]$ ll
total 14428
-rw-r--r--. 1 sandbox users  208148 Jun 26 14:56 765_144hr_test.ang
-rw-r--r--. 1 sandbox users     648 Jun 30 23:43 765_144hr_test_compressionY.C_ref
-rw-r--r--. 1 sandbox users  611455 Jun 30 23:42 765_144hr_test_compressionY_ipbased.vtk
-rw-r--r--. 1 sandbox users  556260 Jun 30 23:42 765_144hr_test_compressionY.mesh
-rw-r--r--. 1 sandbox users  611458 Jun 30 23:42 765_144hr_test_compressionY_nodebased.vtk
-rw-r--r--. 1 sandbox users 3521832 Jun 30 23:58 765_144hr_test_compressionY.out
-rw-r--r--. 1 sandbox users      85 Jun 30 23:43 765_144hr_test_compressionY.outputConstitutive
-rw-r--r--. 1 sandbox users      73 Jun 30 23:43 765_144hr_test_compressionY.outputCrystallite
-rw-r--r--. 1 sandbox users     150 Jun 30 23:43 765_144hr_test_compressionY.outputHomogenization
-rw-r--r--. 1 sandbox users 8975983 Jun 30 23:52 765_144hr_test_compressionY.spectralOut
-rw-r--r--. 1 sandbox users    5320 Jun 30 23:58 765_144hr_test_compressionY.sta
-rw-r--r--. 1 sandbox users   22221 Jun 30 21:44 765_144hr_test.geom
-rw-r--r--. 1 sandbox users  201377 Jun 30 20:53 765_144hr_test.txt
-rw-r--r--. 1 sandbox users      77 Jun 30 23:30 compressionY.load
-rw-r--r--. 1 sandbox users    1165 Jul  1 10:38 do_postprocess.sh
-rw-r--r--. 1 sandbox users   15381 Jun 30 23:19 material.config
[sandbox@materials25 PK03]$ . do_postprocess.sh
```

Run (.) do_postprocess.sh file from this folder (note that it change directory to "postProc"

```
[sandbox@materials25 PK03]$ . do_postprocess.sh

REMARK: h5py module not available

(00:00:28) processing point 2000 of 2262 from increment 15 (position 3)...
```

Postprocessing run may take long…..

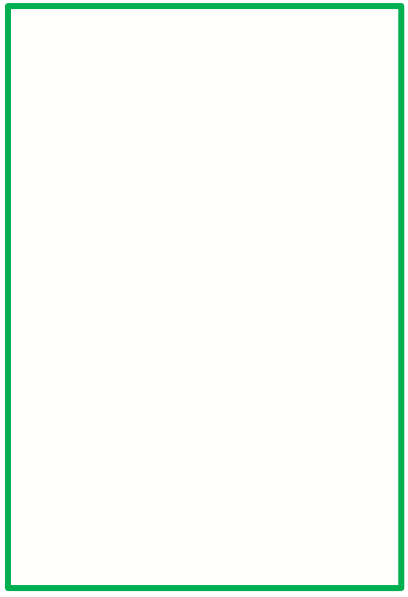


- *Check all text files (notice there names) and corresponding stress, strain, etc. files.*
- *Then transfer all these files from server to your computer using winSCP or something like that*
- *Or, you can "stack" same type of .png files into a animation .gif file (see next slide) – which then can be transferred to your computer*

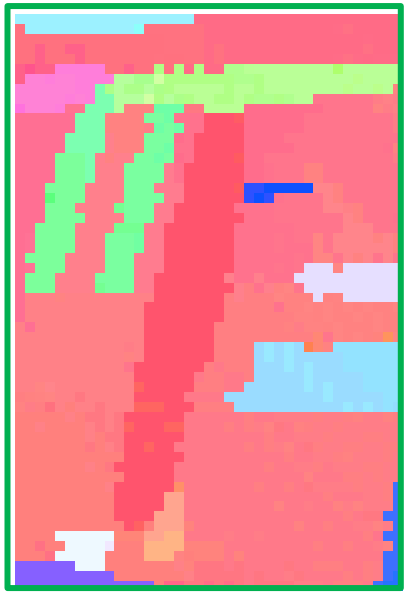
```
-rw-r--r--. 1 sandbox users 1848522 Jul  2 10:04 765_144hr_test_compressionY_inc70.txt
-rw-r--r--. 1 sandbox users    5399 Jul  2 10:04 765_144hr_test_compressionY_inc75_4_grainrotation.png
-rw-r--r--. 1 sandbox users    5220 Jul  2 10:04 765_144hr_test_compressionY_inc75_IPF_001_cubic.png
-rw-r--r--. 1 sandbox users     110 Jul  2 10:04 765_144hr_test_compressionY_inc75_Mises(Cauchy).png
-rw-r--r--. 1 sandbox users    5225 Jul  2 10:04 765_144hr_test_compressionY_inc75_Mises(ln(V)).png
-rw-r--r--. 1 sandbox users 1847819 Jul  2 10:04 765_144hr_test_compressionY_inc75.txt
[sandbox@materials25 postProc]$ convert -set delay 3 *grainrotation*.png GrainRotation.gif
[sandbox@materials25 postProc]$ convert -set delay 3 *IPF*.png IPF_Cubic.gif
[sandbox@materials25 postProc]$ convert -set delay 3 *Cauchy*.png Mises_Cauchy.gif
[sandbox@materials25 postProc]$ convert -set delay 3 *ln(V)*.png Mises_Strain.gif
-bash: syntax error near unexpected token `('
[sandbox@materials25 postProc]$ convert -set delay 3 *ln*.png Mises_Strain.gif
```

Makes a .gif (with 3 s delay between frames) using .png files

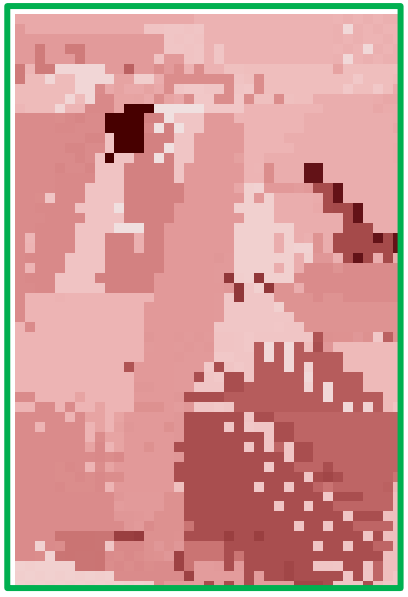
```
-rw-r--r--. 1 sandbox users   45043 Jul  2 10:06 GrainRotation.gif
-rw-r--r--. 1 sandbox users   47051 Jul  2 10:06 IPF_Cubic.gif
-rw-r--r--. 1 sandbox users    1233 Jul  2 10:07 Mises_Cauchy.gif
-rw-r--r--. 1 sandbox users   42498 Jul  2 10:07 Mises_Strain.gif
```



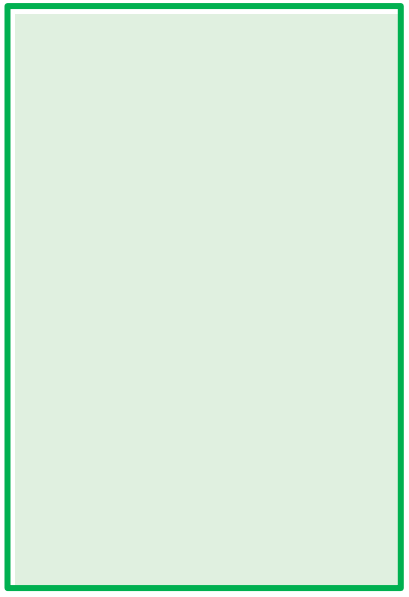
Grain rotation



IPF map



Cauchy stress



Mises strain