


Crystal Application Tutorial: Initial calculations

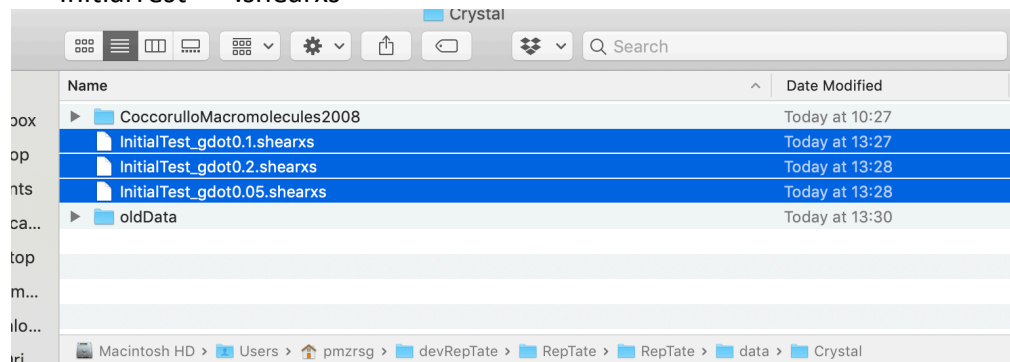
Aim: The tutorial aims to check you have a working version of the Crystal application in RepTate and explore some of the features of the GO-polyStrand model.

Data: The 'data' are all synthetic, meaning they are outputs of the theory. If you use the same model parameters you should be able to perfectly reproduce these data.

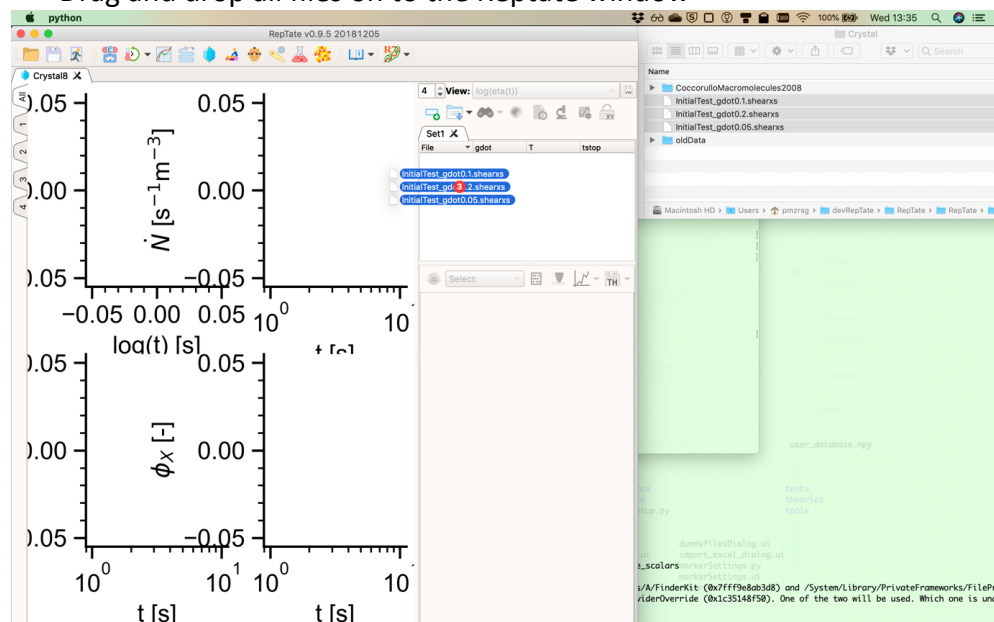
Summary: We will import the synthetic data, run the model to reproduce the calculations and then explore some feature of the model.

Load data

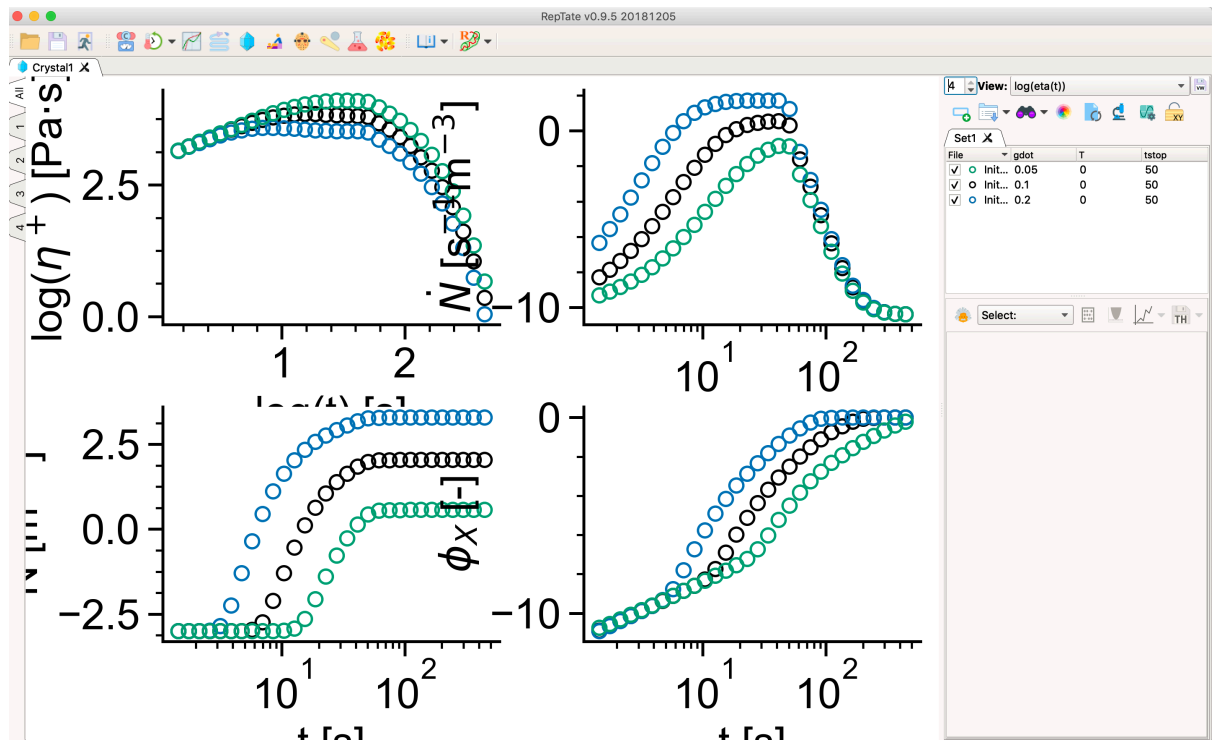
- Load the Crystal application (Click on the crystal application  on the top toolbar)
- Open the folder /RepTate/RepTate/data/Crystal/ and select the 3 files InitialTest***.shearxs




- Drag and drop all files on to the Reptate window

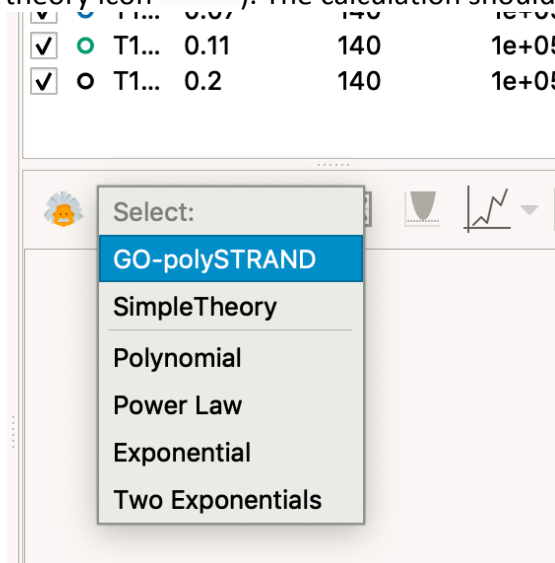


- You should now see

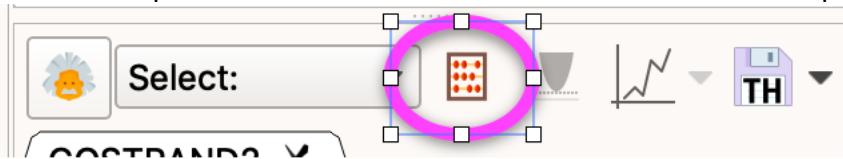


Run the model

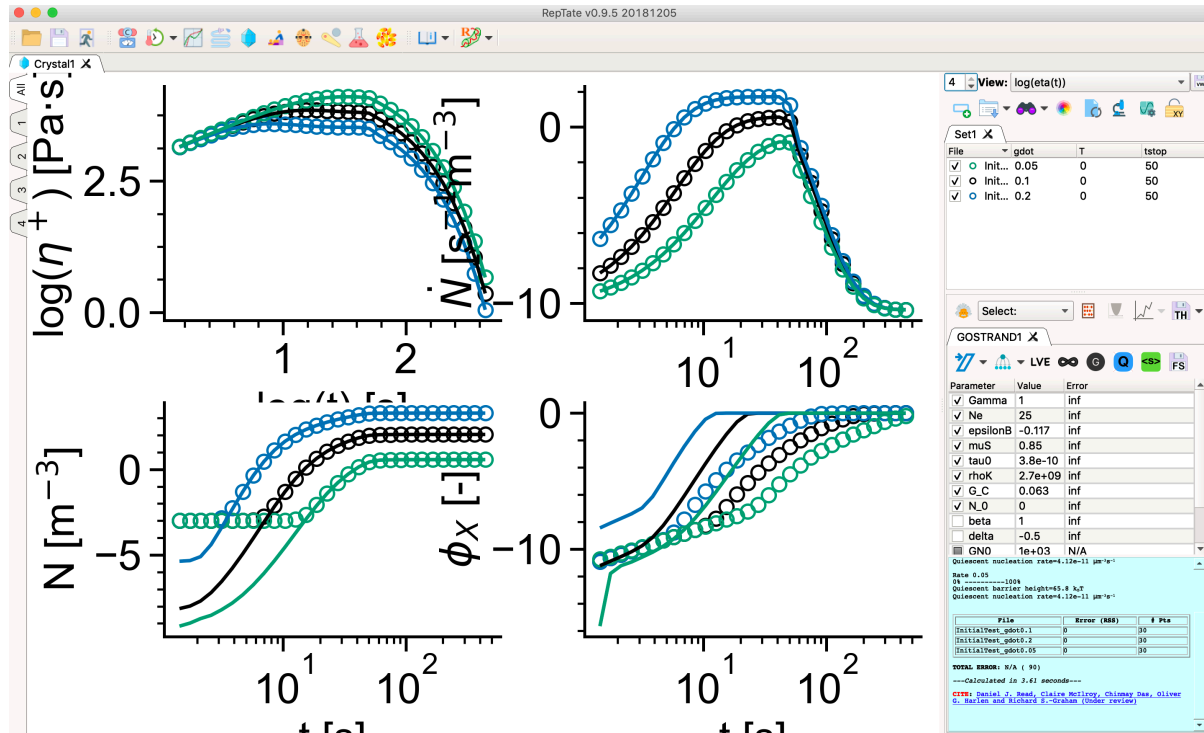
- Load GO-polyStrand model (choose the model from the drop down list and then click the theory icon ). The calculation should take about 4 seconds.



- The default parameters are fine for this calculation so click compute



- You should see



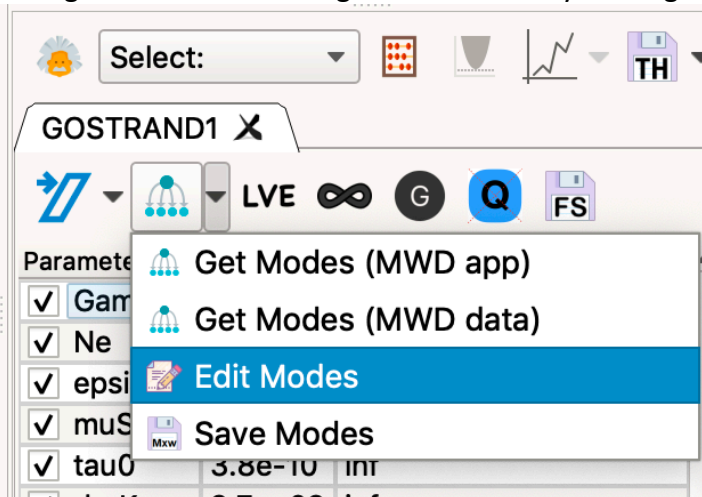
- Set the both parameters G_C and N_0 $1e-3$ to produce full agreement for N and ϕ_x .

<input checked="" type="checkbox"/>	tau0	3.8e-10	inf
<input checked="" type="checkbox"/>	rhoK	2.7e+09	inf
<input checked="" type="checkbox"/>	G_C	0.001	inf
<input checked="" type="checkbox"/>	N_0	0.001	inf
<input type="checkbox"/>	beta	1	inf

Things to try

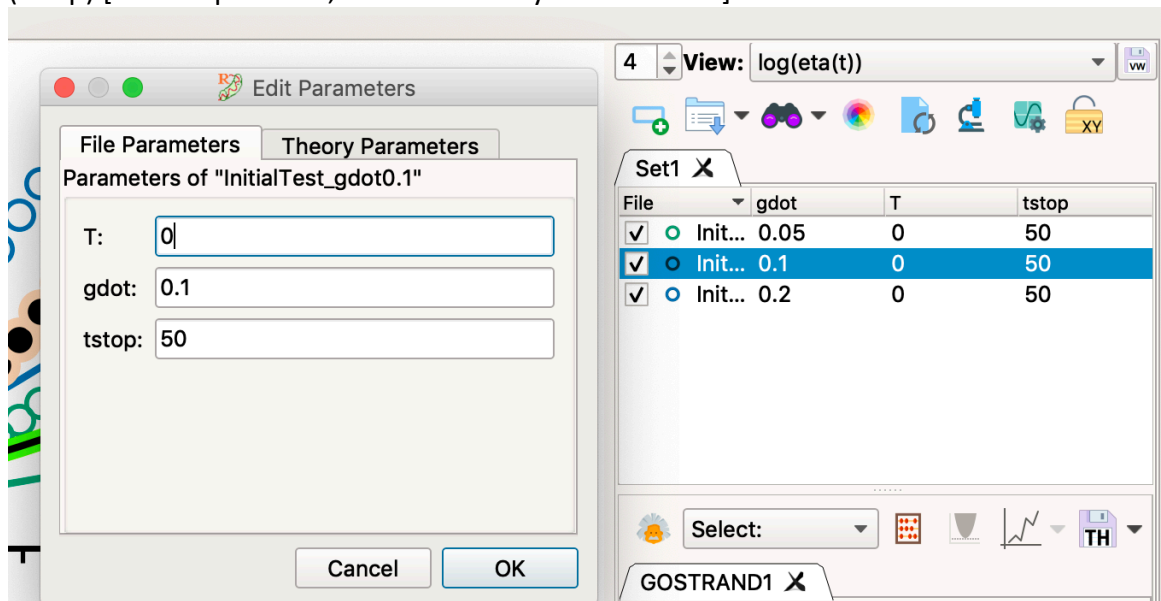
- Change Gamma to adjust the sensitivity to shear
- Make *small* changes to epsilonB to adjust the quiescent barrier (equivalent to changing temperature)
- Adjust tau0 to scale all nucleation rates
- Adjust G_C to change the crystal growth rate

- Change the molecular weight distribution by clicking



and changing the relaxation times, number of modes, and concentrations (this needs to add up to 1).

- Double click on a data set and change the shear rate (gdot) and shear end time (tstop) [T is temperature, which currently has no effect]



- Click the numbered tabs on the left of the screen to make individual plots fill the window



- Use the 'View' menu towards the upper right corner to choose different views.

