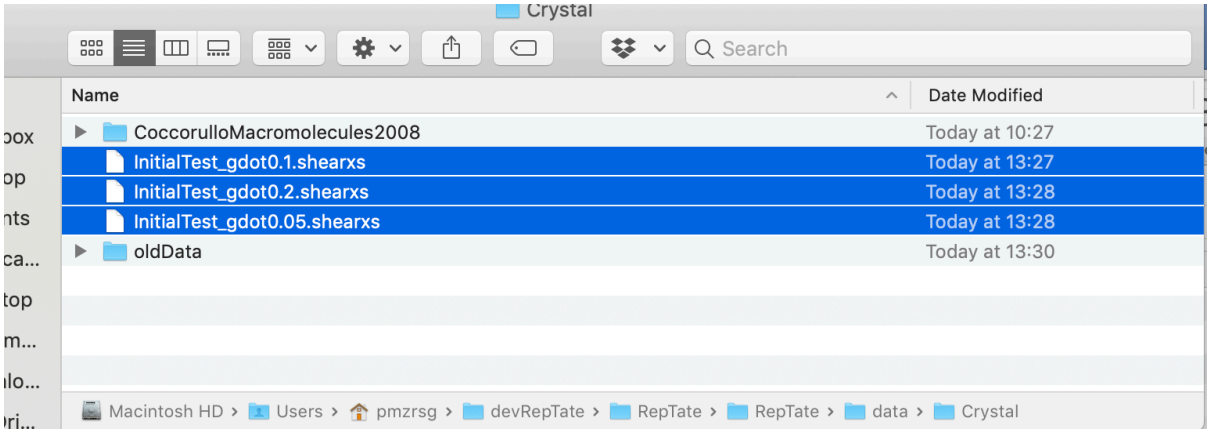
Crystal Application Tutorial: Initial calculations

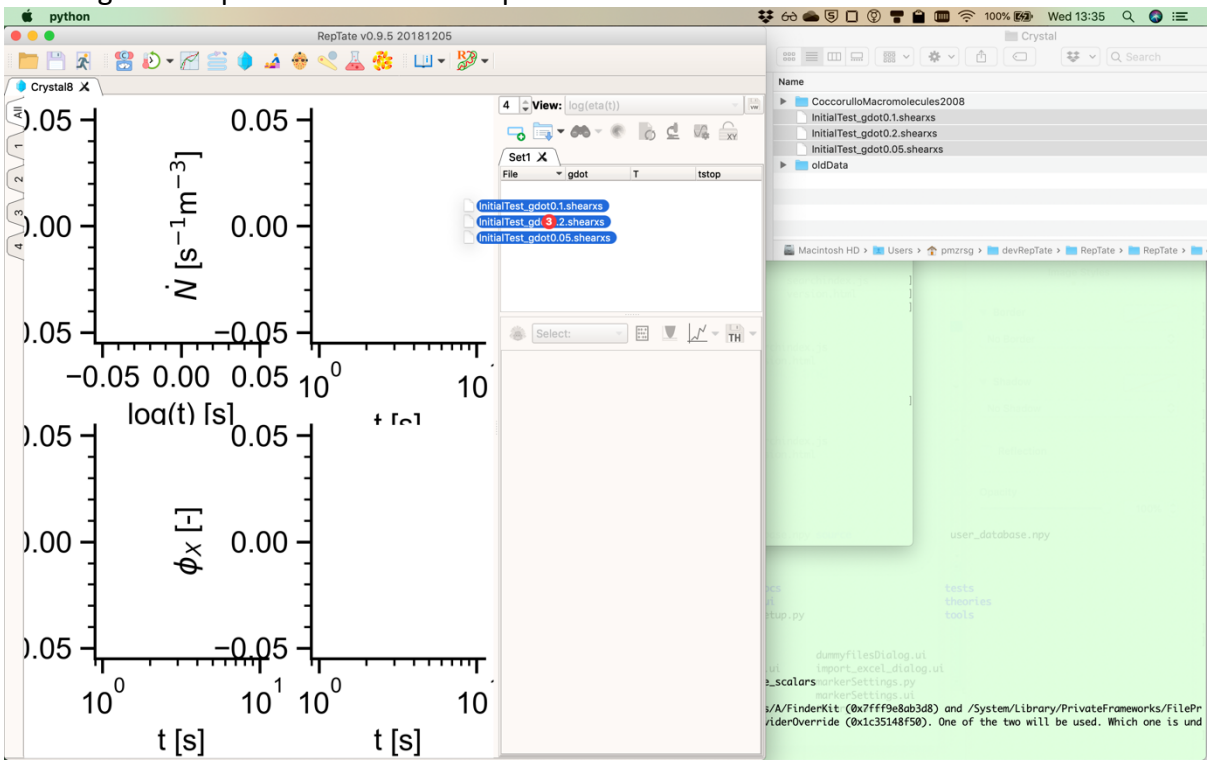
Load data

- Load the Crystal application (Click on the crystal application  on the top toolbar)

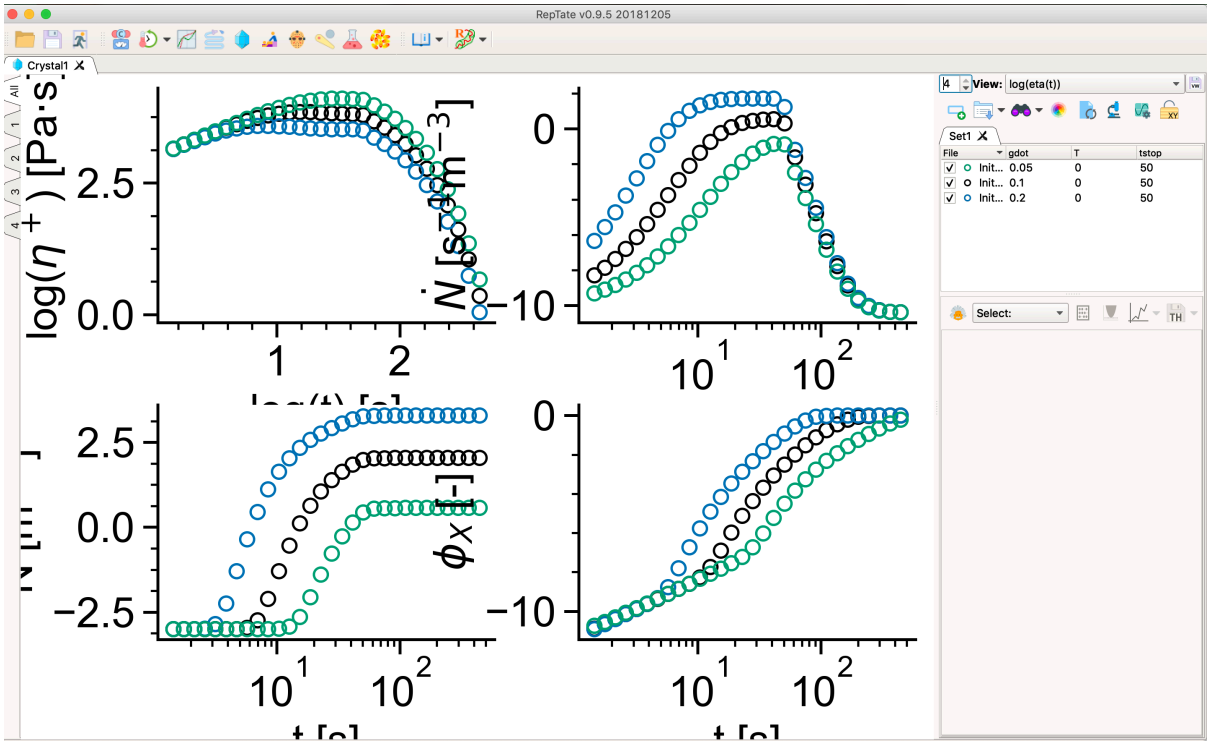
- Open the folder /RepTate/RepTate/data/Crystal/ and select the 3 files InitialTest***.shearxs



- Drag and drop all files on to the Reptate window

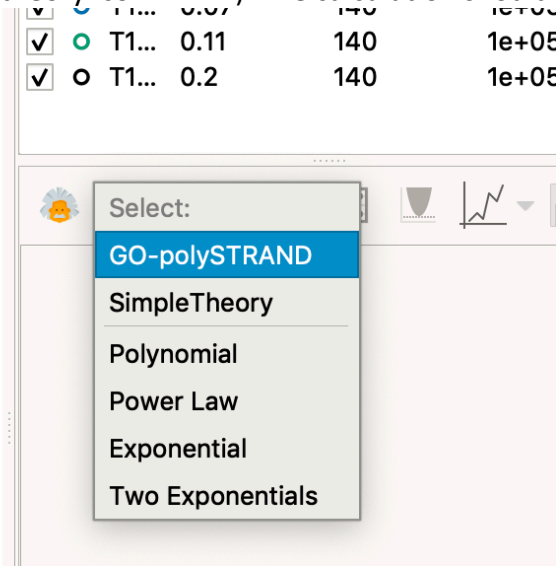


- You should now see

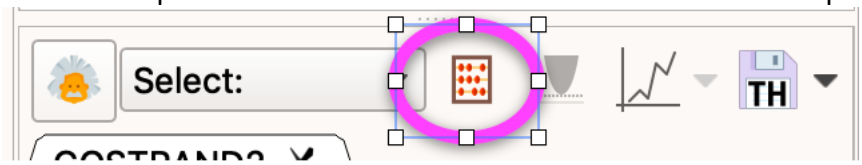


Run the model

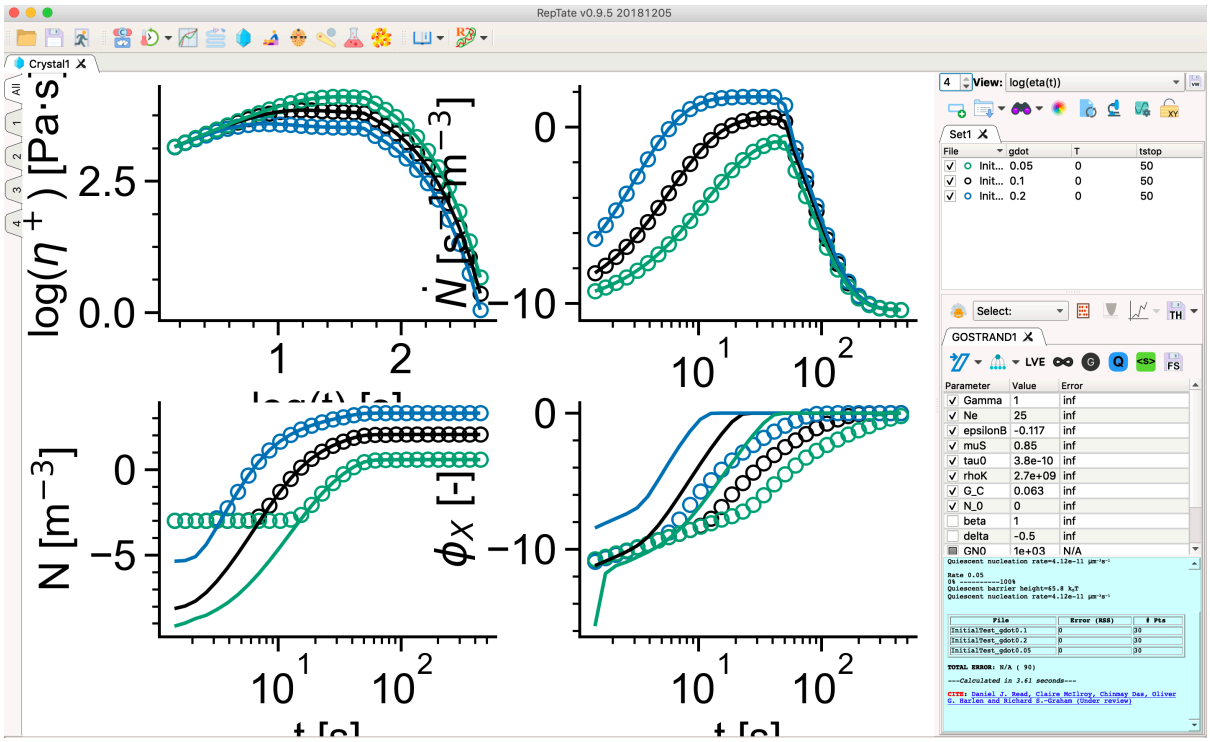
- Load GO-polyStrand model (choose the model from the drop down list and then click the theory icon ). The calculation should take about 4 seconds.



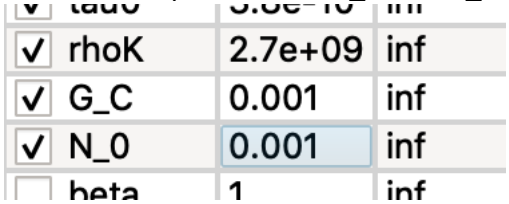
- The default parameters are fine for this calculation so click compute



- You should see



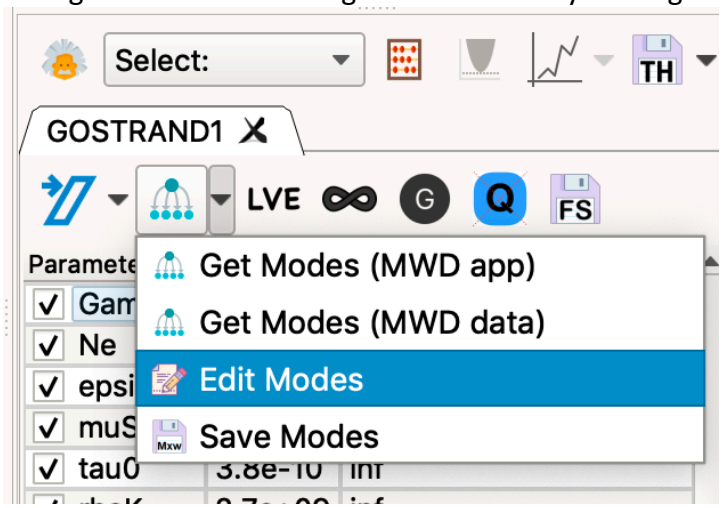
- Set the both parameters G_C and N_0 1e-3 to produce full agreement for N and phi_x.



Things to try

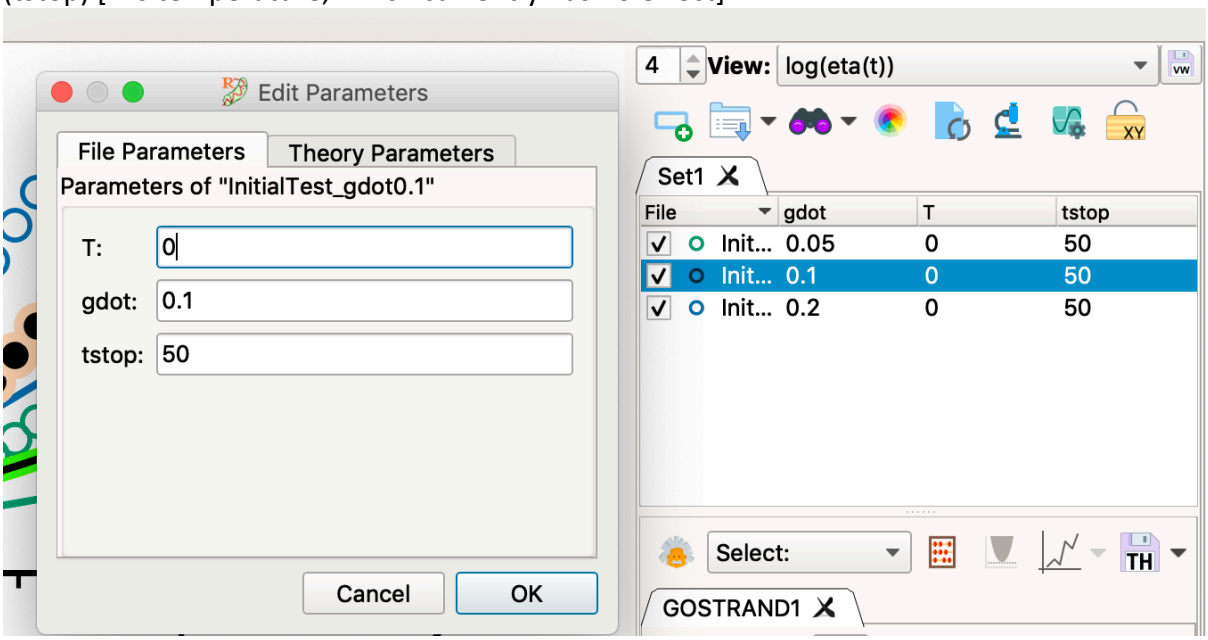
- Change Gamma to adjust the sensitivity to shear
- Make *small* changes to epsilonB to adjust the quiescent barrier (equivalent to changing temperature)
- Adjust tau0 to scale all nucleation rates
- Adjust G_C to change the crystal growth rate

- 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 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.