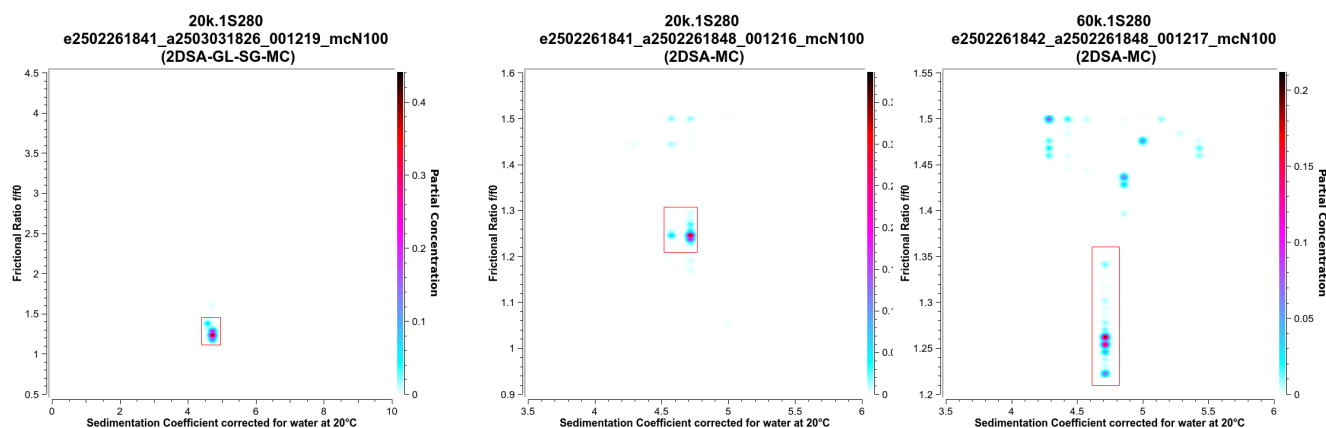


Homework 8:

25 pts. Use the global fitting feature in the LIMS portal to fit the 20k and 60k BSA simulations to a global model. Because you already have all the noise fitted, there is no need to fit any noise anymore. Use the 2DSA method with 100 Monte Carlo iterations. Make sure to check the “Proceed as global fit” radio button is checked when you submit the job.

25 pts. Load the superglobal 2DSA-Monte Carlo model into the “Velocity:Initialize Genetic Algorithm” module and draw a box around the strongest signal (see below) and click “Save” and “View Statistics”. Take a screenshot of the graph for the superglobal GL-SG-2DSA-MC model, the 20k 2DSA-MC, and the 60k 2DSA-MC model, and show how you drew the integration box. Compare the 95% confidence intervals for the three conditions. Indicate which condition has the most narrow confidence interval for s , as well as for D and f/f_0 , and explain why.



25 pts: For the global models, compare the RMSD values of the SC, SG, and VR models for 20k and 60k. Please note that the SG model can be used for both 20k and 60k runs. To locate the SG model, in the genetic algorithm initializer program, do not pick a PreFilter, and search for “SG” in the search box. The SG model will only be associated with one of the speeds, which depends on the sequence in which you loaded them into the fitter. In the “Velocity:Finite Element Model Viewer”, unclick “Filter by Edit/Run” and put “SG” into the “Search” field. Show a matrix like this:

60k: 0.0058865 (SC)
20k: 0.00558073 (SC)
60k: 0.00588268 (VR)
20k: 0.0055802 (VR)
60k: 0.00590116 (SG)
20k: 0.00559489 (SG)

Based on the RMSDs shown in your matrix, what properties about the samples can you derive? Explain.

Homework is due on Sunday, 3/9