**SIMULATION**

**1. Identify pericentromeric regions to split chr1 into arms**

Up to you if you want to repeat Zahra, I think two weeks is okay given that I’m still waiting for 4.2.

Hg38 – bins 3043-3580

**Hg19 – bins 3038-3565**

**I will be masking 3039-3563, gap common in 21 tissues**

**2. Key parameters**

a. Cut-off – <2 is fine

b. Parameter set for 3.2 and 4.2 – just use 10\_5

Is it a parameter set specific for implementing attractive force based on complementarity?

Not applicable for cp=21 contacts, Set2?

c. Arm-interaction type

Interacting and non-interacting for 3.2 and 4.2

Set2 (cp only) – why no non-interacting version?

For non-interacting of 3.2, did you exclude cp=21 between arms?

d. c|| - categorised or not? - **categorised**

e. Ask about force field changes that decreased number of contacts from around 25% to less than 1%?

**3. Normalisation of frequency maps**

Simulation maps contain frequency of contact not distance. Maps are generated for roughly 72 hours but different timescales (until it converges).

Normalise to number of snapshots taken during equilibrium.

**4. Replicates – can be done if not at the expense of waiting time; getting the average of replicates increases robustness given that replicates behave the same.**

**Minimum required normalised final matrices**

**1. (1) Set1 – I**

**2. (2) Set2 – I**

**3. (2) Set3.2 – I and NI x cut-off <2 x parameter 10\_5**

**4. (2) Set4.2 - I and NI x cut-off <2 x parameter 10\_5**

**I choose parameters to lessen the matrices generated but if this is something that you can run at the same time Zahra (two weeks), I don’t see the problem with running other parameters to prepare for reviewer comments.**

**Also, I’m making these suggestions without full details of the simulation, so final decisions up to you ☺**