Star polymers provide insight on Rabl-like chromosome conformations

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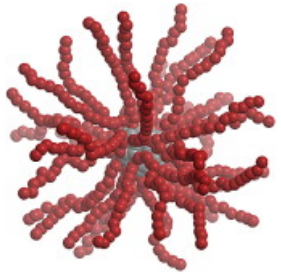
Second Annual MIT PRIMES Conference, May 20, 2012

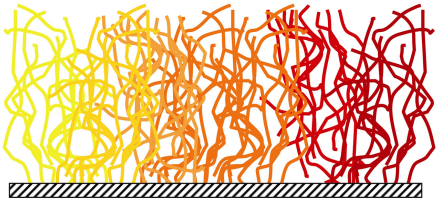
Background

Star polymers: polymers that are bound together at a point



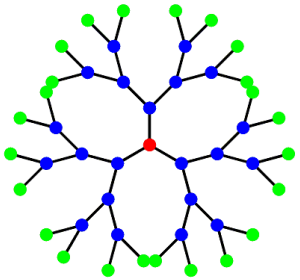
Solomon 2003

Brush polymers: polymers bound to a backbone



Bello 2006

Dendritic polymers: polymers with a repeated branching pattern

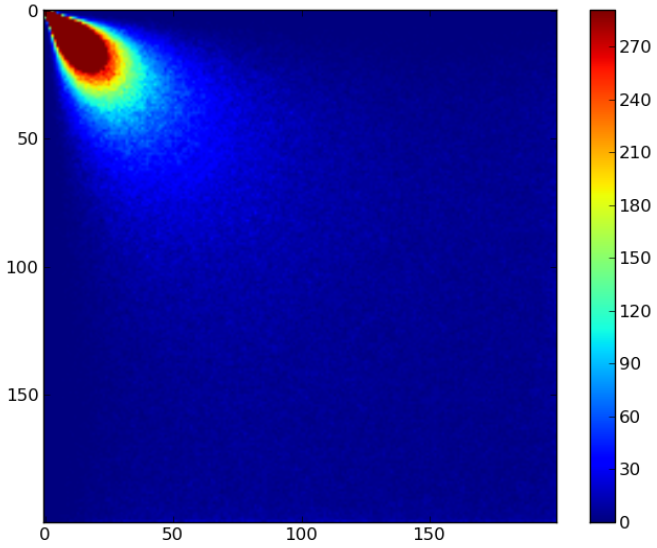


Chow 2012

Background

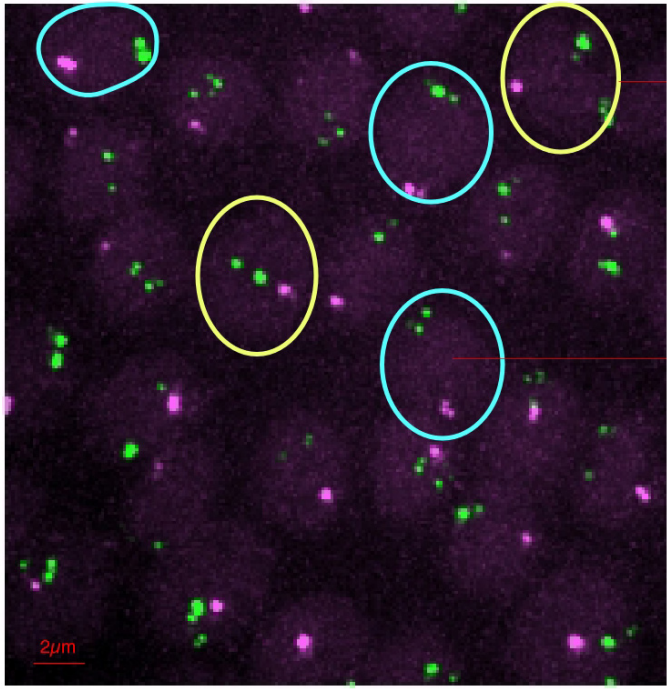
Averaged Contact Map: heat map of all contact points averaged over many states

Heat Map: a graphical representation of values in colors

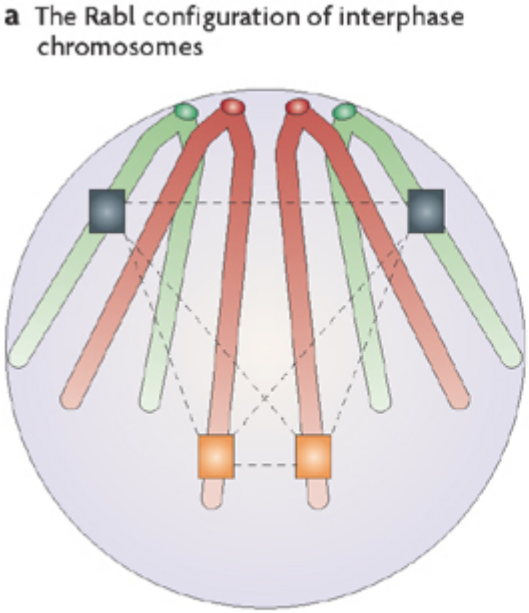


Biological implications for star polymers: Yeast Chromosomes

Rabl Formations in Yeast Cells:

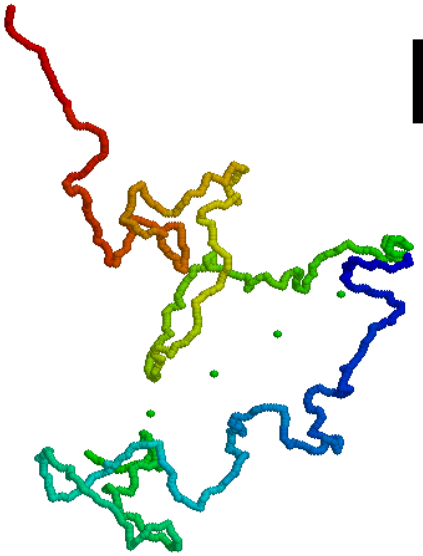


Cell Science 2006

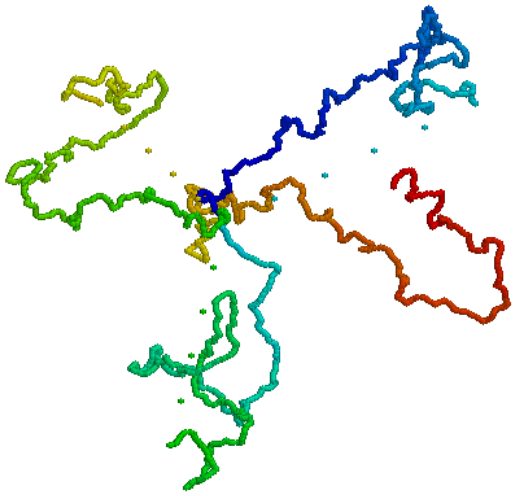


Barzel 2008

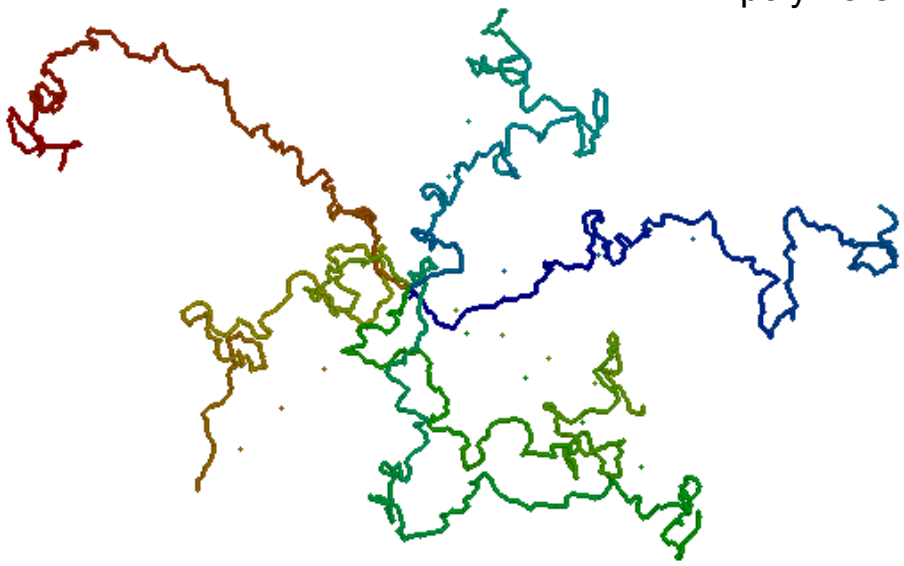
Models



2 polymers



4 polymers



6 polymers

Goal

To study the pattern of interactions between two arms in a star polymer

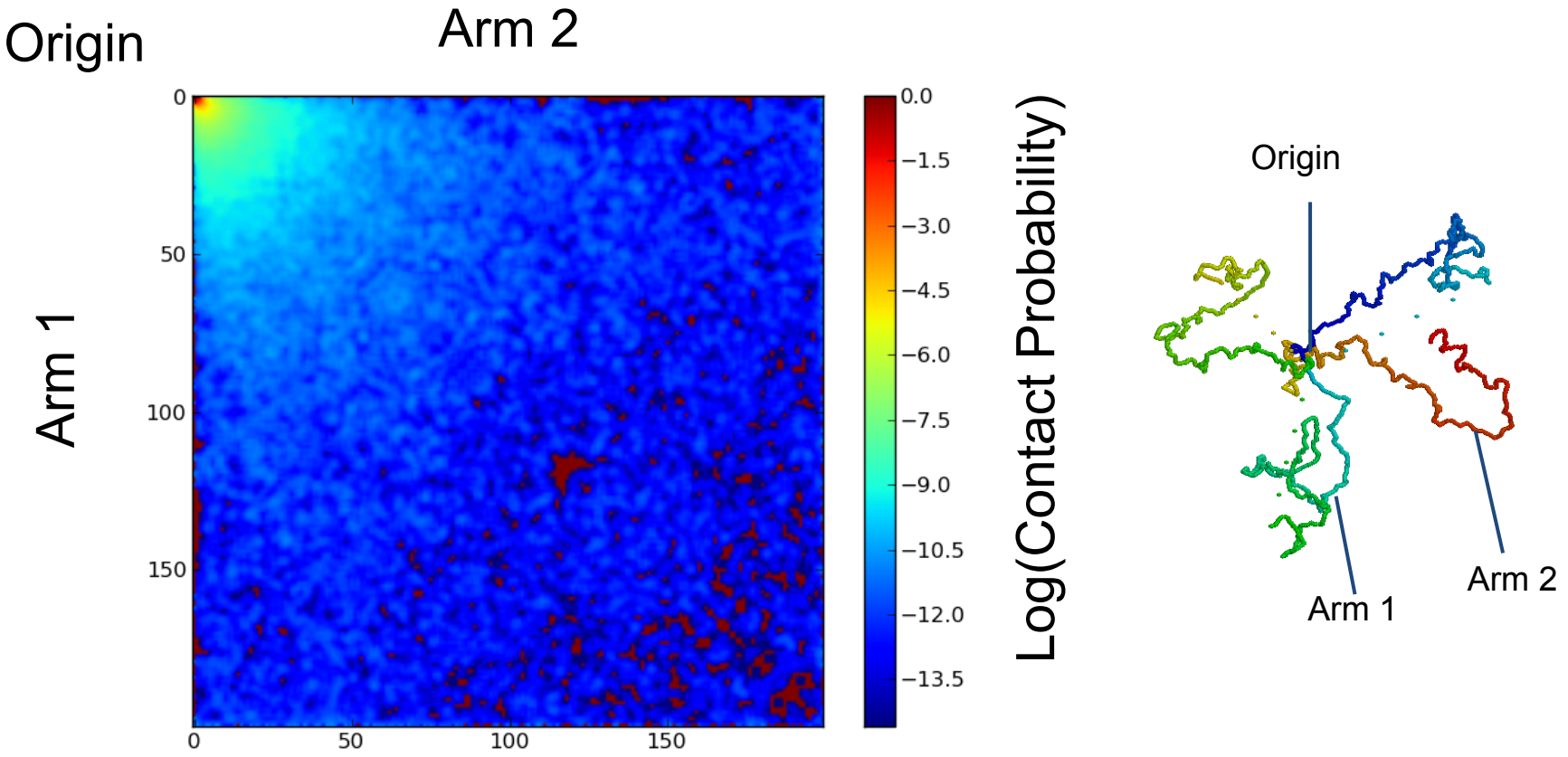
Method: simulate and create contact maps of star polymers (with various numbers of arms)

My programs

1. Creating the system:
   slice a long coiling polymer
   rotate and translate slices to origin
   tether to origin
2. Simulating star-polymers over long times
   use Brownian (Molecular) Dynamics
   collect simulation data
3. Analyzing the simulations:
   Take in contact maps and output contact probabilities
   compare two contact maps
   create cross sections

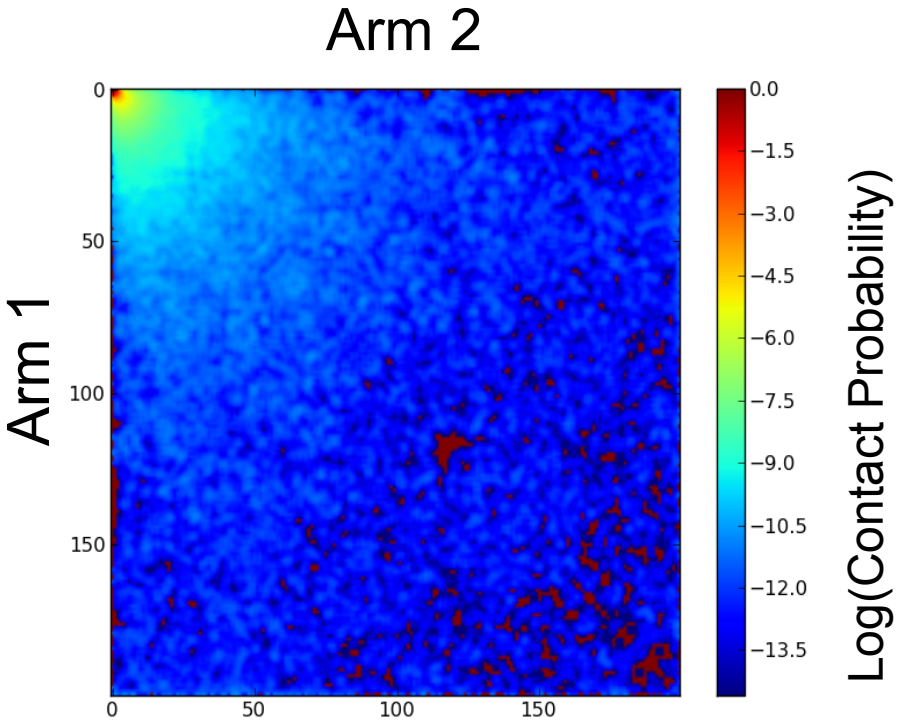
Results

Between-Arm Contact Probability in a 4-Arm Star Polymer

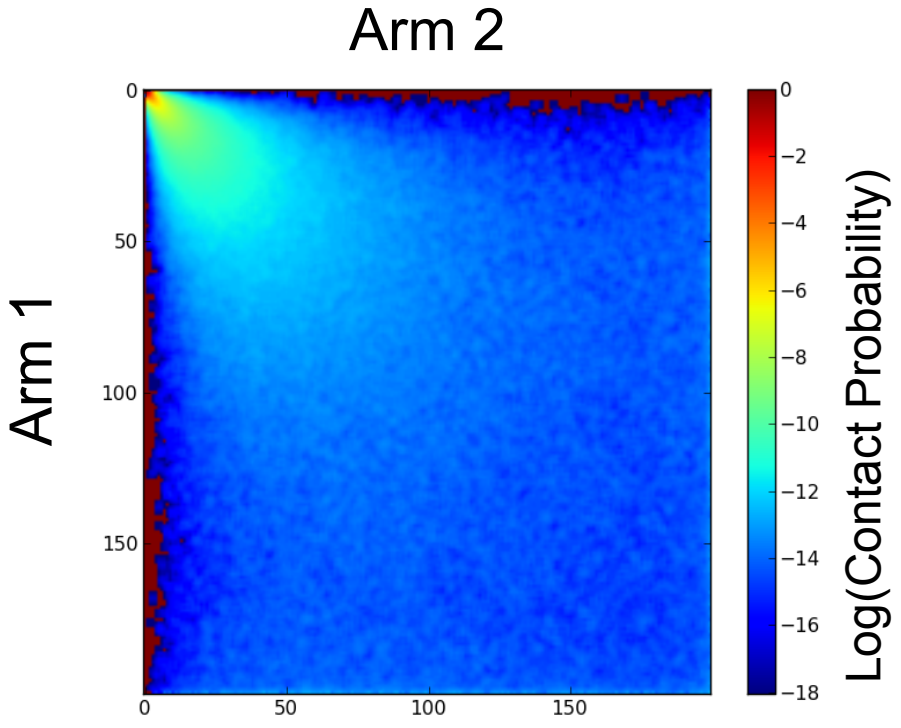


Results: arms in a many-arm star polymer run away parallel to each other

4-arm star polymer

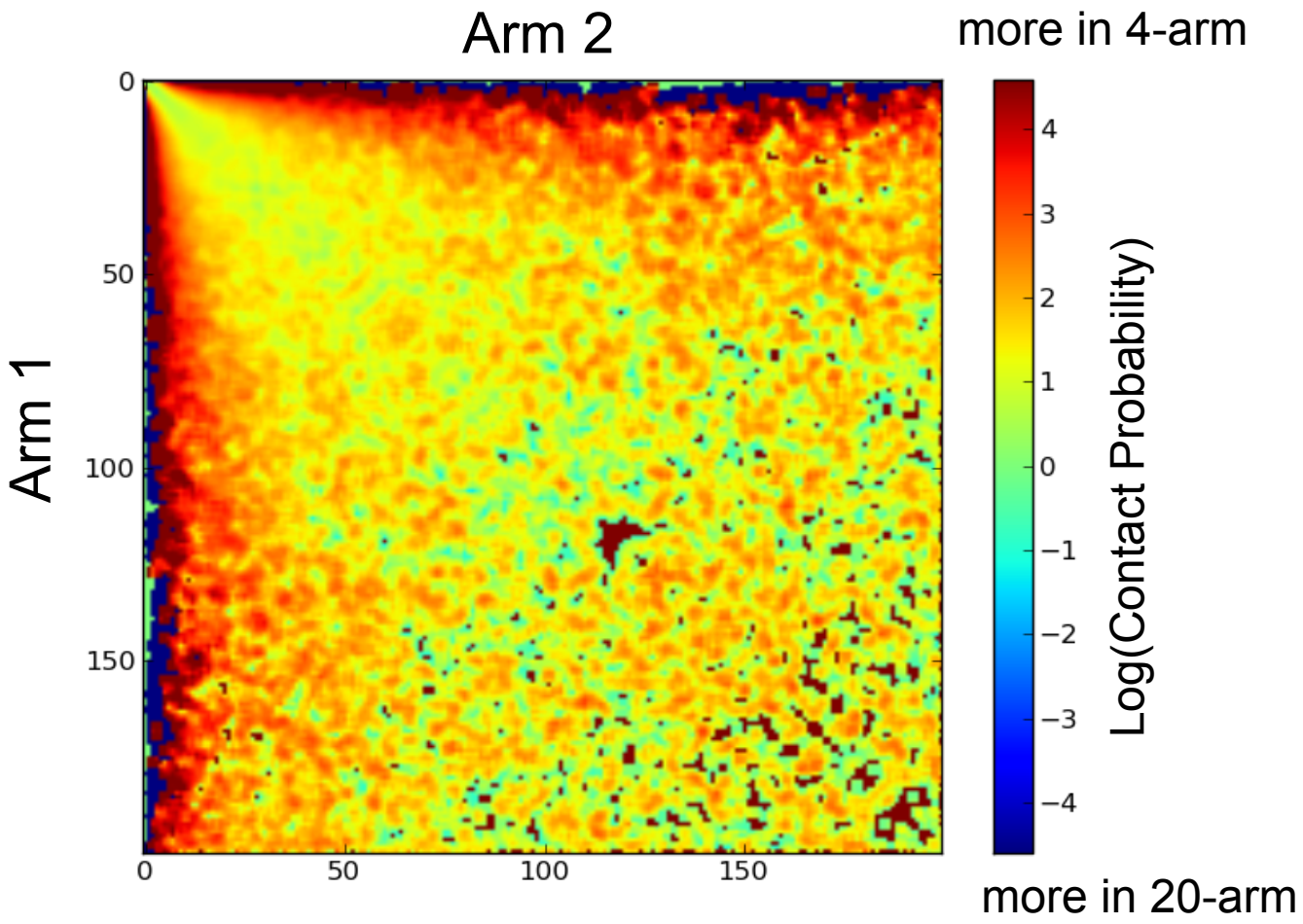


20-arm star polymer



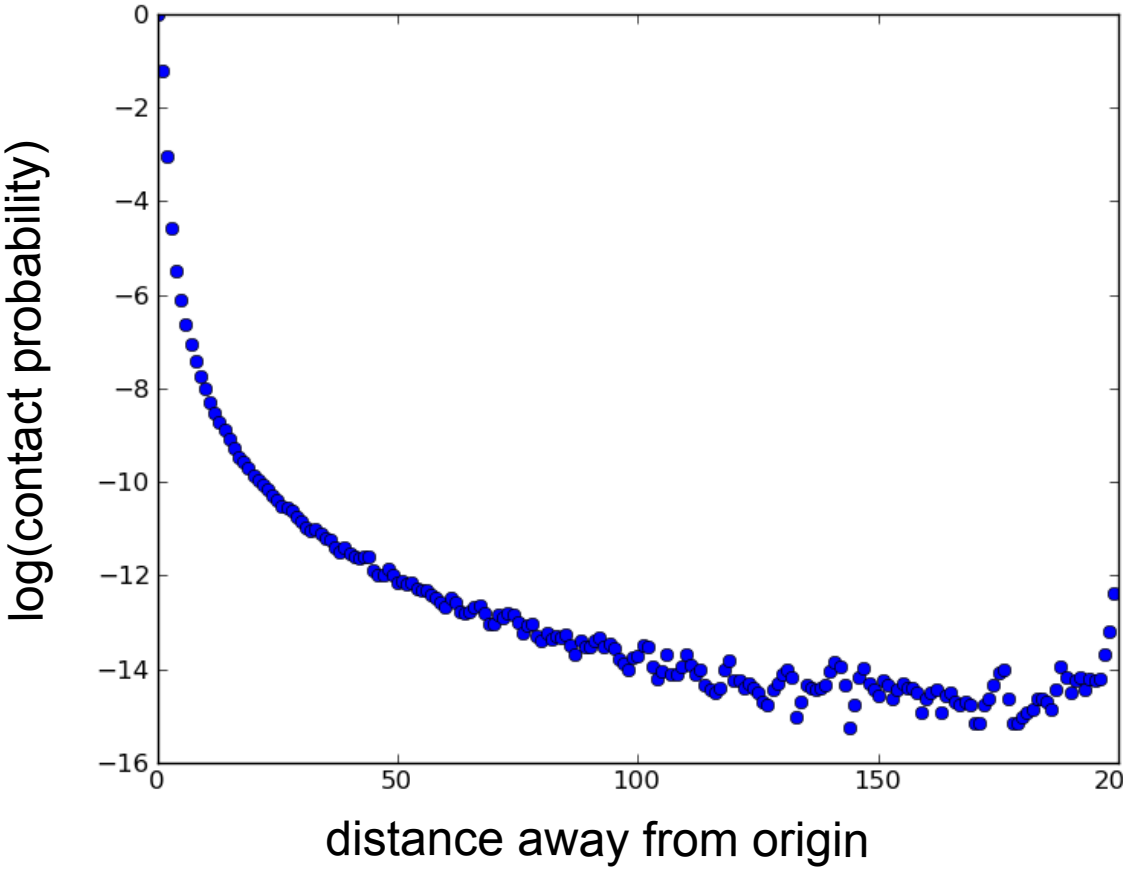
Results

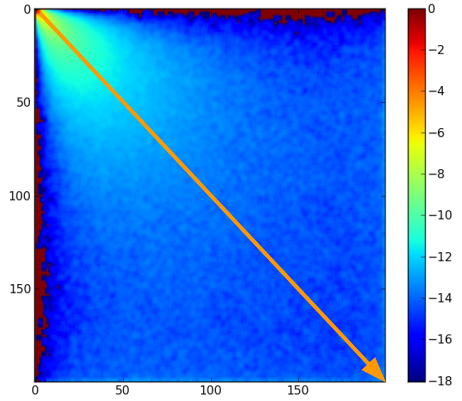
Contact Probability Difference Between 4-arm and 20-arm star polymers

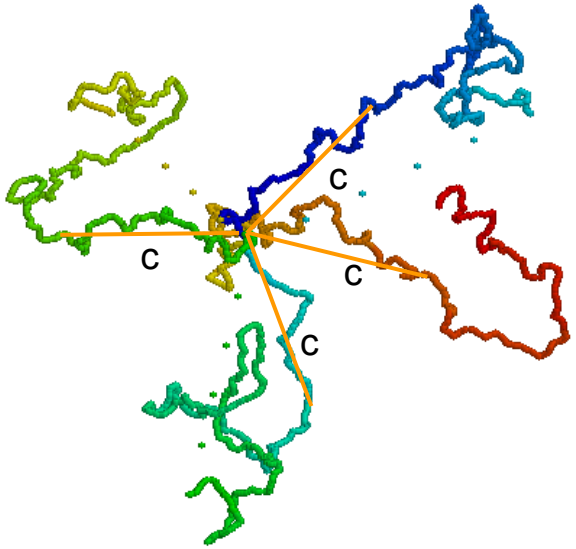


Results: contact probability decays with distance from the origin

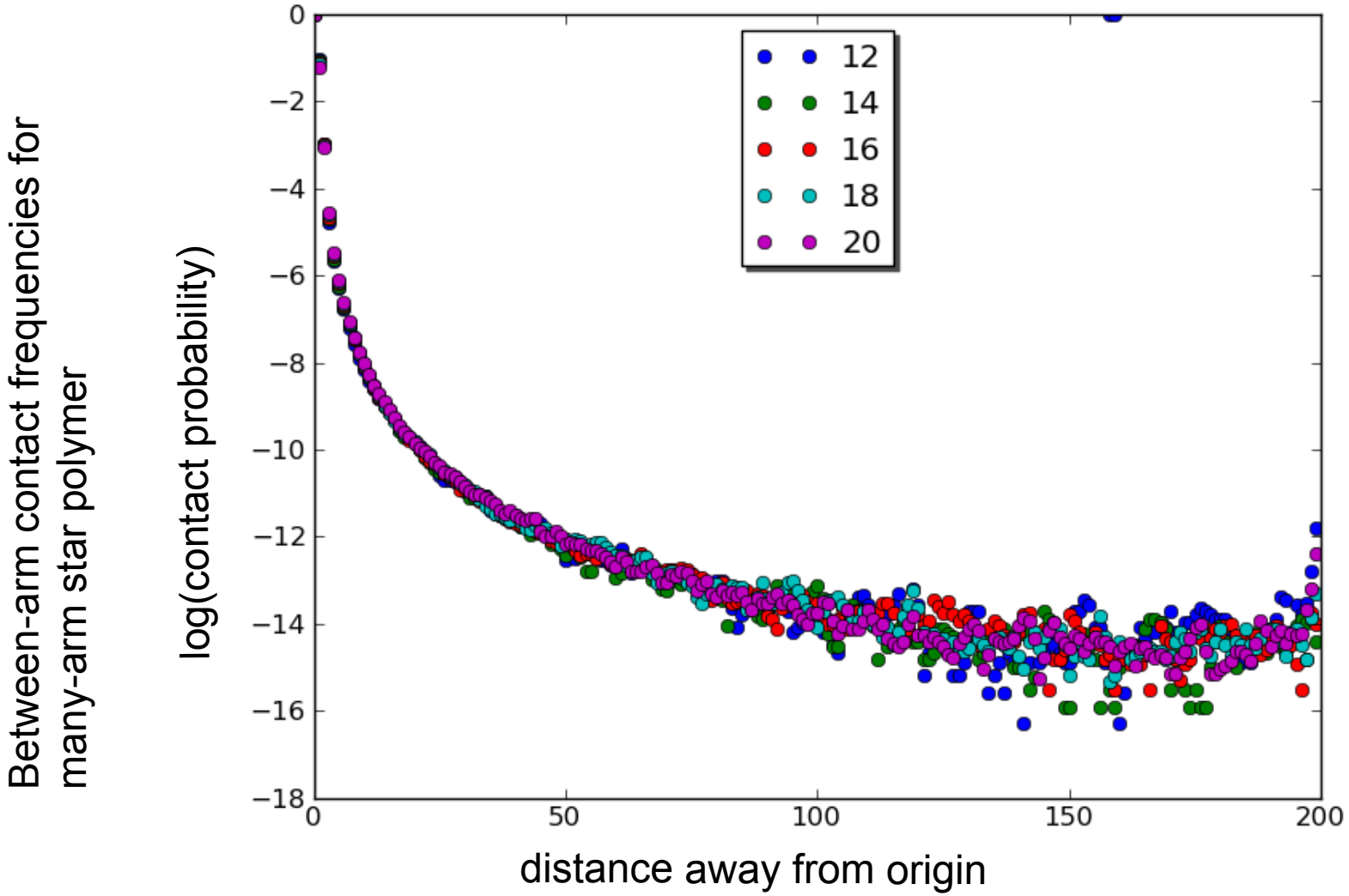
Between-arm contact frequencies for 20-arm star polymer





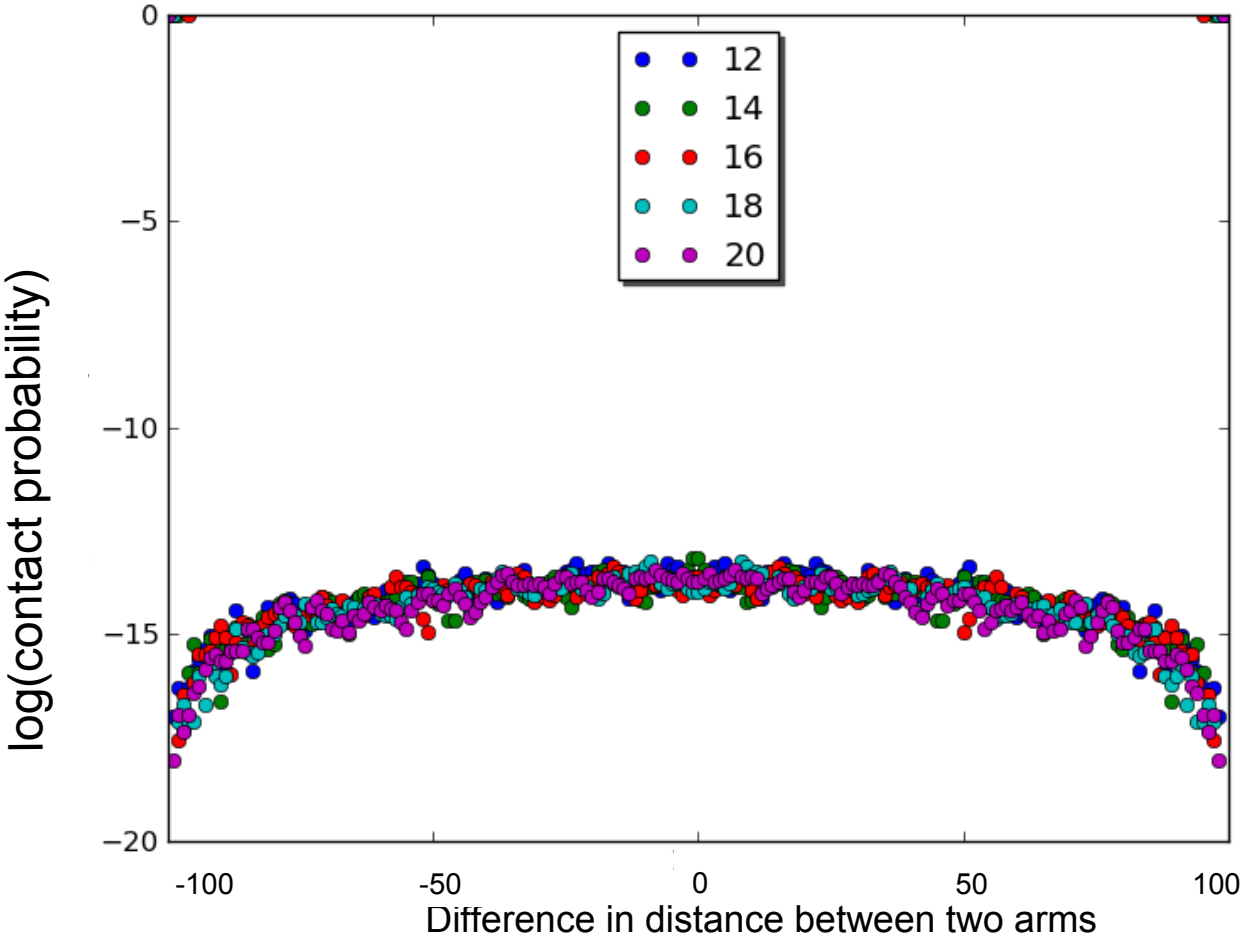


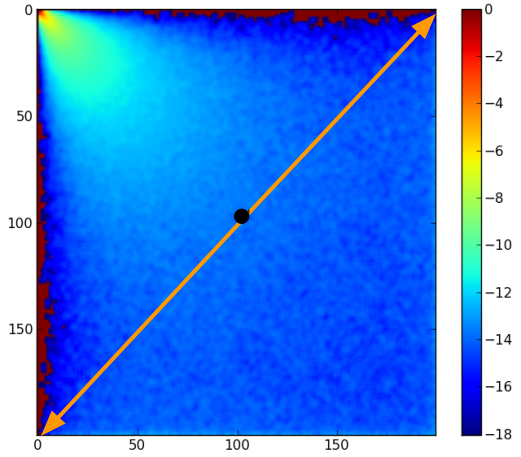
Results: decay of contact probability from origin is remarkably similar for different numbers of arms



Results: contact probability is similar for arms away from the origin

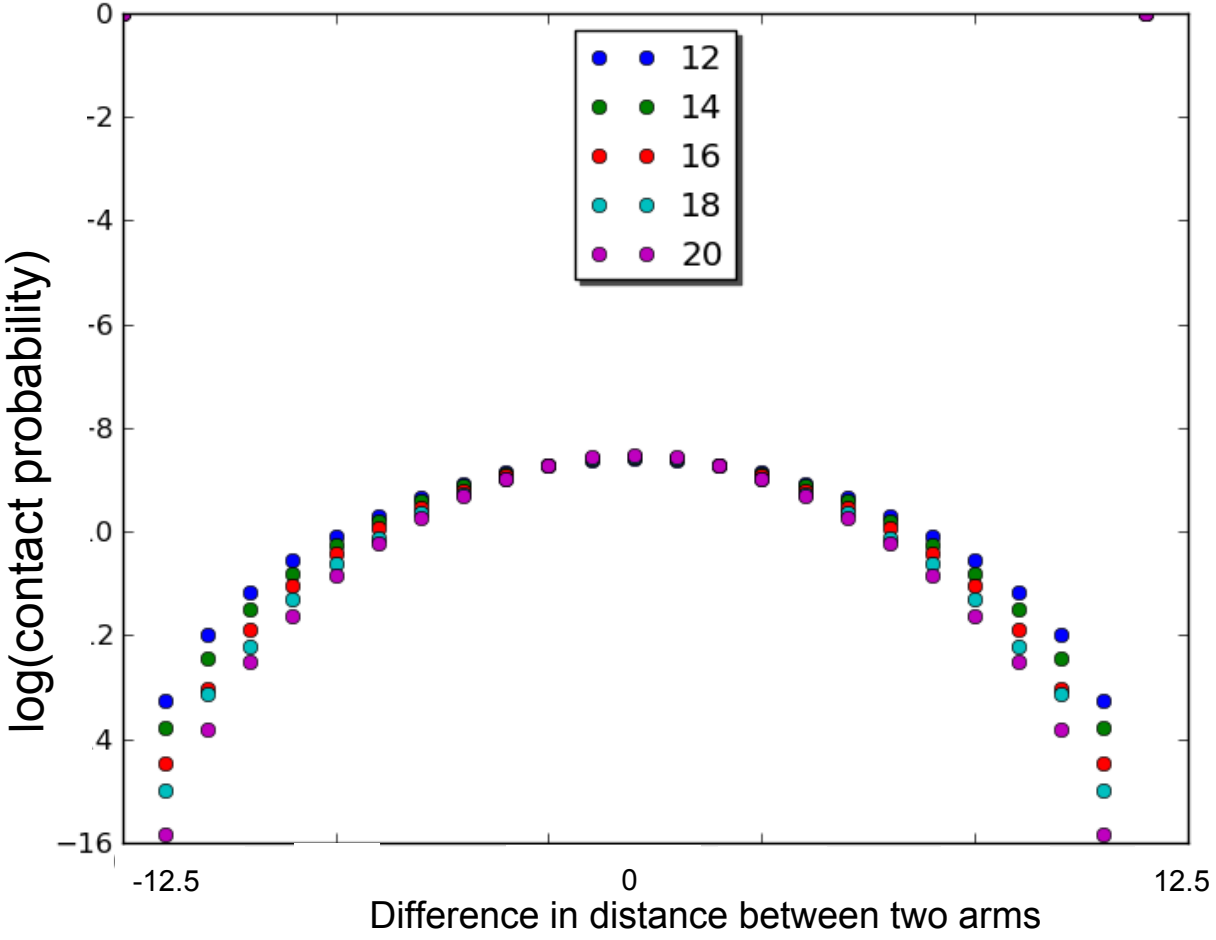
Between-arm contact frequencies at a combined distance of 200 from the origin

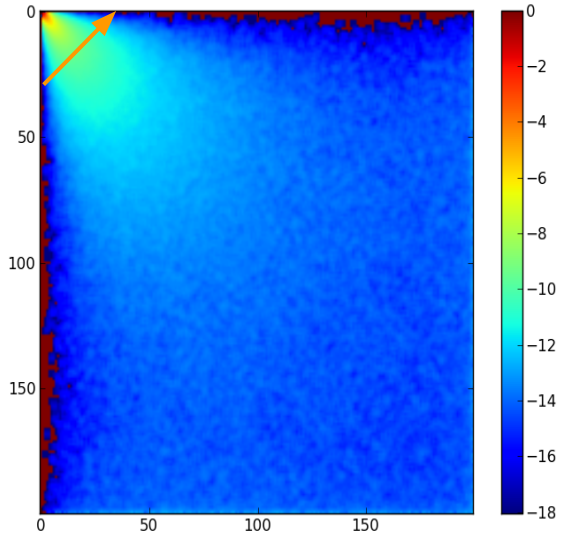




Results: contact probability varies more with more arms in regions close to the origin

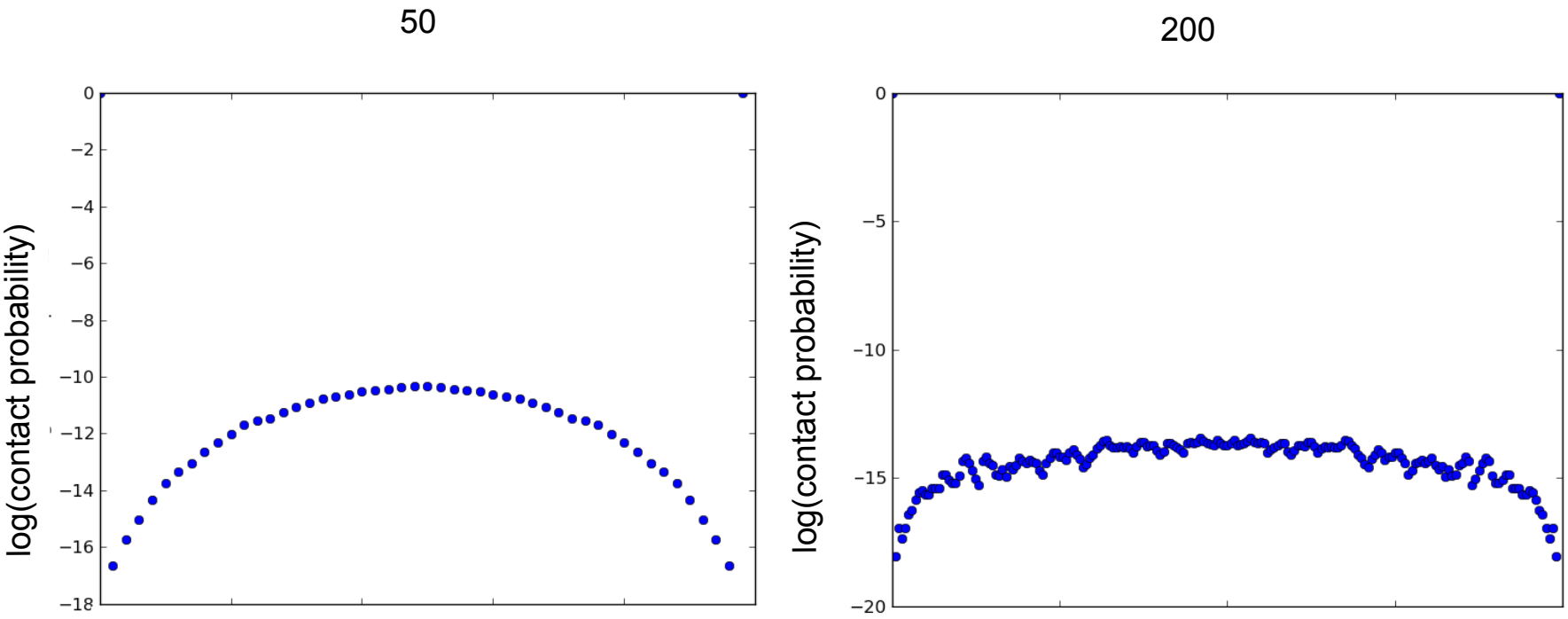
Between-arm contact frequencies at a combined distance of 25 from the origin



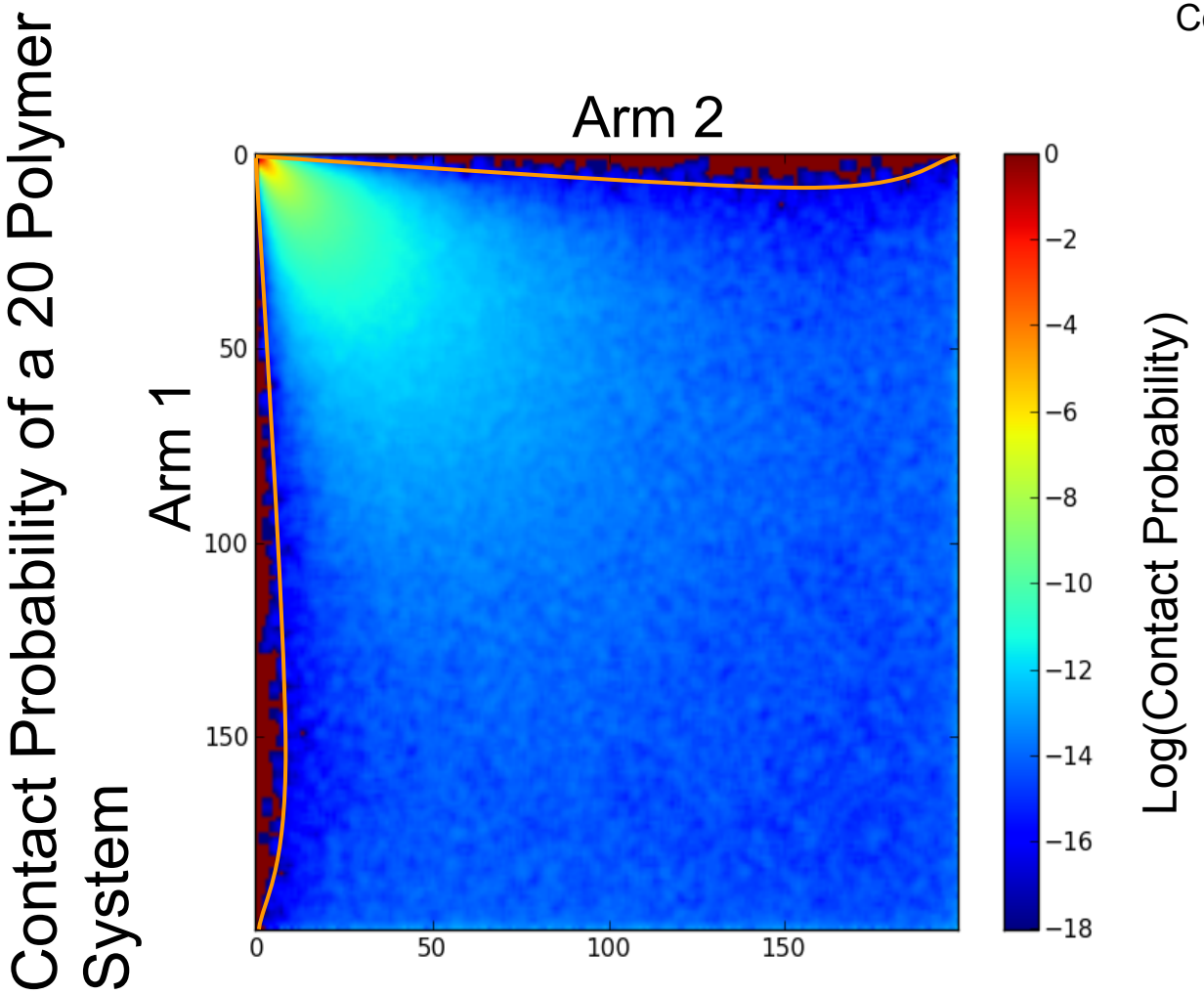


Results: contact probabilities vary more closer to origin

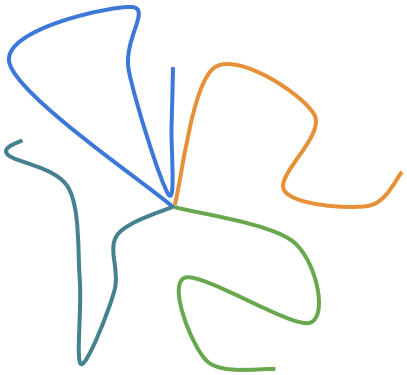
Difference in between-arm contact frequencies at a combined distance of 50 and 200 from the origin



Results: End of polymer tends to loop back to origin more easily than middle of polymer



Contact between middle and origin



Contact between end and origin

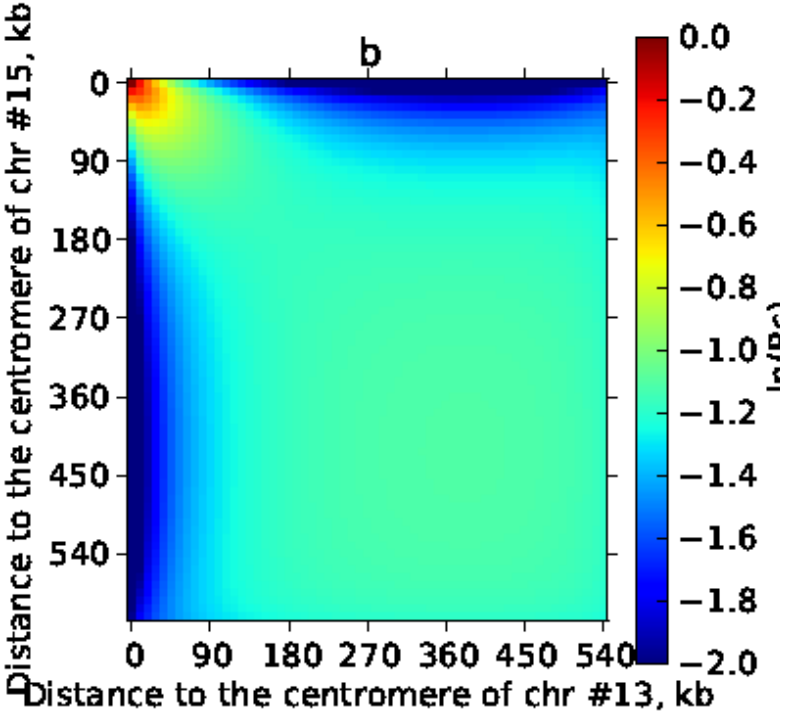
Results show similarities with theoretical models

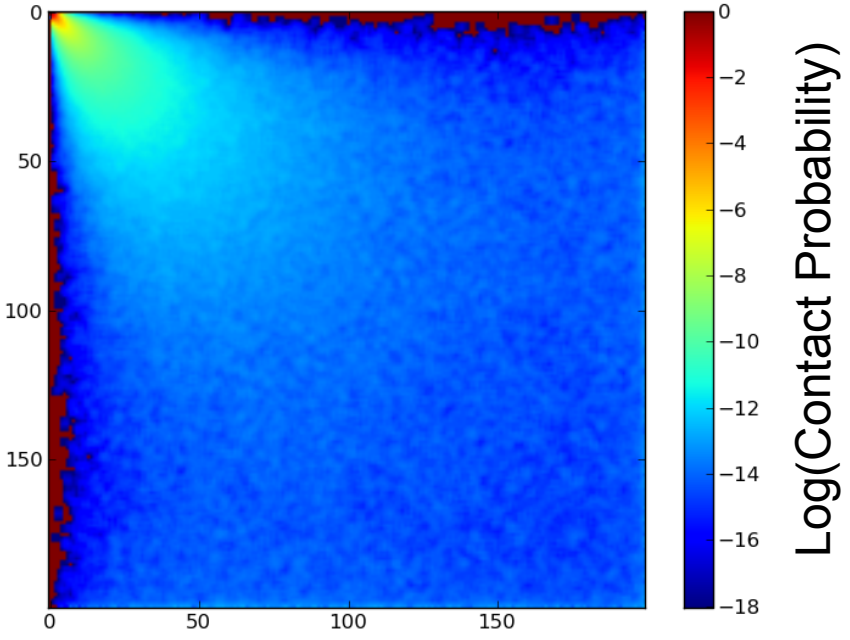
Theoretical Contact Map

My Simulation

32-arm Star Polymer

20-arm Star Polymer





Acknowledgements

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- Professor Leonid Mirny