

SUPPLEMENTARY MATERIAL for Negri *et al.* – Spontaneous domain formation in disordered copolymers as a mechanism for chromosome structuring

S1. ENTROPY OF A DISORDERED STAR POLYMER

The goal of this section is to calculate the the free energy of a star polymer, which is proportional to the total number of blobs N_{blob} ,

$$\beta F = N_{\text{blob}} , \quad (\text{S1})$$

where $\beta = 1/k_{\text{B}}T$.

Hypotheses

We refer to the sketch in Fig. S3. In the case of a regular star, we picture the semidilute region as made of concentric spherical shells of thickness $\xi(r)$, each crossed by f arms. This means that each shell is made of f blobs of dimension $\xi(r)$.

From these assumptions we can write an expression for ξ based on the condition that the volume of one shell, divided by f , must equal the volume of a blob. Consequently, we can write

$$\frac{r^2 \xi}{f} = \xi^3$$

and then the expression for the blob size ξ :

$$\xi(r) = f^{-1/2} r. \quad (\text{S2})$$

To account for the different length of the arms, we consider the number of arms f as a decreasing function of the radius, $f(r)$. We give an ansatz for this function

$$f(r) = f_0 \left(\frac{r}{b} \right)^{-\gamma} , \quad (\text{S3})$$

where b is the radius of the core of the star and $\gamma \geq 0$.

Combining eq. S2 and eq. S3 we obtain the relation between blob size and radial coordinate r ,

$$\xi(r) = f_0^{-1/2} b \left(\frac{r}{b} \right)^{1+\frac{\gamma}{2}} . \quad (\text{S4})$$

Positions of the shells

We are interested in the radial coordinate of each shell r_m , because, as we will see, we can relate it to the monomer concentration. Since the thickness of a shell is $\xi(r)$, we can relate the radii of two

consecutive shells with the following rule:

$$r_{m+1} - r_m = \xi(r_m) ,$$

which can be approximated to a simple differential equation

$$\frac{dr(m)}{dm} = \xi(r(m))$$

whose solution, using the expression in eq. S4, is

$$r(m) = b \left[1 - \frac{\alpha}{2} f_0^{-1/2} m \right]^{-\frac{2}{\gamma}} \quad (\text{S5})$$

for $\gamma \neq 0$.

If $\gamma = 0$, i.e. in the case of the regular star, the solution is exponential,

$$r(m) = b e^{f_0^{-1/2} m}. \quad (\text{S6})$$

Monomer concentration

Since a blob behaves by definition as a swollen polymer, its dimension is related to the number of monomers g it contains by $\xi = a g^\nu$, where a is the distance between two consecutive monomers. We set $\nu = 3/5$. Therefore we invert this relation and we use eq. S4 to obtain $g(r)$:

$$g(r) = \left(\frac{\xi(r)}{a} \right)^{5/3} = \left(f_0^{-1/2} \frac{b}{a} \right)^{5/3} \left[\frac{r}{b} \right]^{\frac{5}{3}(1+\frac{\gamma}{2})} \quad (\text{S7})$$

Given the number of monomers in one blob $g(r)$, we can calculate the radial monomer concentration $c(r)$ from the total number of monomers in one shell divided by the volume of the shell,

$$c(r) = \frac{f(r)g(r)}{4\pi r^2 \xi(r)}.$$

Using eq. S3, S4 and S7 this equation gives the dependency of the monomer concentration from the radial coordinate,

$$c(r) = \frac{1}{4\pi r^2} \frac{1}{b} f_0^{2/3} \left(\frac{b}{a} \right)^{5/3} \left[\frac{r}{b} \right]^{\frac{2}{3}(1-\gamma)}. \quad (\text{S8})$$

Radius of the star polymer

Since we know the total number of monomers N_{tot} in the star polymer, we can now integrate the concentration to obtain an expression of the radius R of the star polymer,

$$\begin{aligned} N_{tot} &= \int_b^R 4\pi r^2 c(r) dr \\ &= f_0^{2/3} \left(\frac{b}{a} \right)^{5/3} \int_b^R \left[\frac{r}{b} \right]^{\frac{2}{3}(1-\gamma)} \frac{dr}{b} = \end{aligned}$$

$$= f_0^{2/3} \left(\frac{b}{a} \right)^{5/3} \frac{3}{5-2\gamma} \left[\left(\frac{R}{b} \right)^{\frac{5-2\gamma}{3}} - 1 \right]. \quad (\text{S9})$$

Now we observe that we must exclude $\gamma > 5/2$, because it corresponds to an inverse relation $R(N_{\text{tot}})$ that diverges for a certain finite value of N . So we set $\gamma < 5/2$ and we invert the relation S9 to obtain $R(N_{\text{tot}})$,

$$R(N_{\text{tot}}) = b \left(1 + \frac{5-2\gamma}{3} \left(\frac{a}{b} \right)^{5/3} f_0^{-2/3} N_{\text{tot}} \right)^{\frac{3}{5-2\gamma}}.$$

We can neglect the term $+1$ in the parentheses since we consider the second term much greater than 1,

$$R(N_{\text{tot}}) \simeq b \left(\frac{5-2\gamma}{3} \left(\frac{a}{b} \right)^{5/3} f_0^{-2/3} N_{\text{tot}} \right)^{\frac{3}{5-2\gamma}}. \quad (\text{S10})$$

The above expression gives the radius of the star polymer, which we now need to use to compute the total number of blobs.

Number of shells

We evaluate $r(S)$ using eq. S5, where S is the total number of shells in the star polymer; then we compare it to the expression S10 for R :

$$r(S) \equiv R.$$

Now we can finally obtain an expression for S

$$b \left[1 - \frac{\gamma}{2} f_0^{-1/2} S \right]^{-\frac{2}{\gamma}} = \left(\frac{5-2\gamma}{3} \left(\frac{a}{b} \right)^{5/3} f_0^{-2/3} N_{\text{tot}} \right)^{\frac{3}{5-2\gamma}}.$$

This leads to

$$S = \frac{2}{\gamma} f_0^{1/2} \left[1 - \left(\frac{5-2\gamma}{3} \left(\frac{a}{b} \right)^{5/3} f_0^{-2/3} N_{\text{tot}} \right)^{-\frac{\gamma}{2} \frac{3}{5-2\gamma}} \right]. \quad (\text{S11})$$

We observe that this expression reduces to the one for the regular star polymer [?] in the limit $\gamma \rightarrow 0$

$$S \sim f_0^{1/2} \log \left[\left(\frac{5}{3} \left(\frac{a}{b} \right)^{5/3} f_0^{-2/3} N_{\text{tot}} \right)^{-\frac{3}{5}} \right] \quad (\text{S12})$$

where we used the limit formula

$$\lim_{\gamma \rightarrow 0} \frac{x^\gamma - 1}{\gamma} = \log x$$

Number of blobs

In order to finally obtain the expression for the number of blobs in the star, we need to calculate the series

$$N_{\text{blob}} = \sum_{m=1}^S f(r_m). \quad (\text{S13})$$

For $f(r_m)$, we combine the expression of the scaling of f

$$f(r) = f_0 \left(\frac{r}{b} \right)^{-\gamma}$$

and the expression of the radius of the m -th shell

$$r(m) = b \left[1 - \frac{\gamma}{2} f_0^{-1/2} m \right]^{-\frac{2}{\gamma}}.$$

We obtain

$$f(r(m)) = f_0 \left[1 - \frac{\gamma}{2} f_0^{-1/2} m \right]^2.$$

Plugging this last equation into eq. S13 we find

$$\begin{aligned} N_{\text{blob}} &= \sum_{m=1}^S f_0 \left[1 - \frac{\gamma}{2} f_0^{-1/2} m \right]^2 \\ &= \sum_{m=1}^S f_0 \left[1 - \gamma f_0^{-1/2} m + \frac{\gamma^2}{4} f_0^{-1} m^2 \right]. \end{aligned}$$

Approximating the series with an integral we obtain the simplified expression

$$N_{\text{blob}} \simeq f_0 \left[S - \gamma f_0^{-1/2} \frac{S^2}{2} + \frac{\gamma^2}{4} f_0^{-1} \frac{S^3}{3} \right] \quad (\text{S14})$$

Again we observe that in the limit $\gamma \rightarrow 0$ this expression reduces to the one for the regular star

$$N_{\text{blob}} \simeq (f_0)^{3/2},$$

since we drop the logarithmic term in equation S12.

Discussion on the ansatz

In order to justify the ansatz S3 on the scaling of the number of blob per shell, this section shows how $f(r)$ can be linked to the distribution $p(N)$ of the number of monomers in a single arm. In particular we will find that, given a certain value of the exponent γ , there is a power law distribution $p(N)$ that produces $f(r) = f_0(r/b)^{-\gamma}$.

In order to perform this estimate, we interpret $f(r)$ as the fraction of arms that reach *at least* a distance r from the core; namely $f(r)$ is the probability that one arm arrives at least at a distance r . This probability is nothing but the cumulative distribution of the probability $p(r)$ that one arm reaches the distance r ,

$$f(r) = 1 - \int_0^r p(r') dr'.$$

We can thus obtain the probability $p(r)$ taking the first derivative of the cumulative distribution:

$$p(r) = -\frac{\partial}{\partial r} f(r). \quad (\text{S15})$$

Since we are interested in the probability as a function of the number of monomers N , we need to change the variable, obtaining

$$p(N) = p(r) \left(\frac{dN}{dr} \right)^{-1} \bigg|_{r(N)}, \quad (\text{S16})$$

To find the number of monomers contained in a sphere of radius r , $N(r)$, we integrate the number $g(r)$ of monomers in one blob

$$N(r) = \int_b^r g(r') dr',$$

where $g(r) = (f(r)^{-1/2}r)^{1/\nu}$. Furthermore we observe that

$$\frac{dN}{dr} = g(r).$$

Thanks to these relations, the expression S16 becomes

$$p(N) = f'(r)(f(r)^{-1/2}r)^{1/\nu} \quad (\text{S17})$$

Plugging the ansatz S3 into the equation S17, we find the expression of the number of monomers contained in a sphere of radius r

$$N(r) \sim r^{\frac{1}{\nu}(1+\frac{\gamma}{2})+1}$$

and the expression of the probability that one arm has N monomers

$$p(N) \sim r(N)^{-1-\gamma-\frac{1}{\nu}(1+\frac{\gamma}{2})}. \quad (\text{S18})$$

Using the equation S17 into the expression in eq. S18, we finally obtain probability distribution of arm lengths $p(N)$ that corresponds to our ansatz for the decay of the number of arms $f(r) = f_0(r/b)^{-\gamma}$,

$$p(N) \sim N^{-1-\frac{\gamma}{\frac{1}{\nu}(1+\frac{\gamma}{2})+1}}. \quad (\text{S19})$$

S2. SUPPLEMENTARY FIGURES

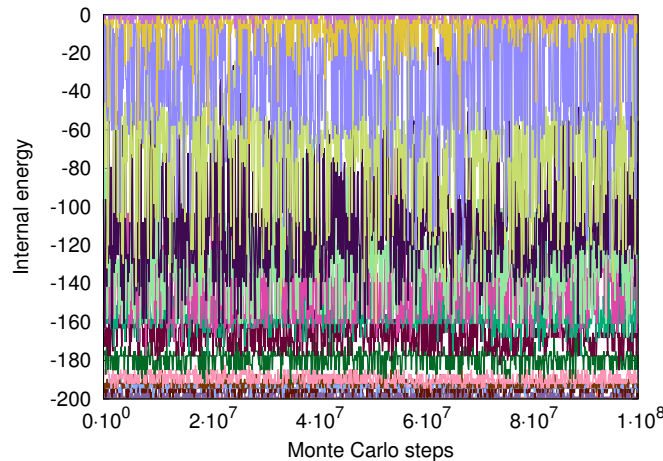


Fig. S1: Each replica must have its energy overlapping with the energy of the contiguous ones, so that the different replicas can exchange configuration. The plot shows we show the MC trajectories of energy in the typical situation at equilibrium (we show only half of the replicas for visual clarity).

Simulations were performed with $N = 513$, $R = 1.44$, $\lambda = 1.42$ for 3×10^9 Monte Carlo sweeps.

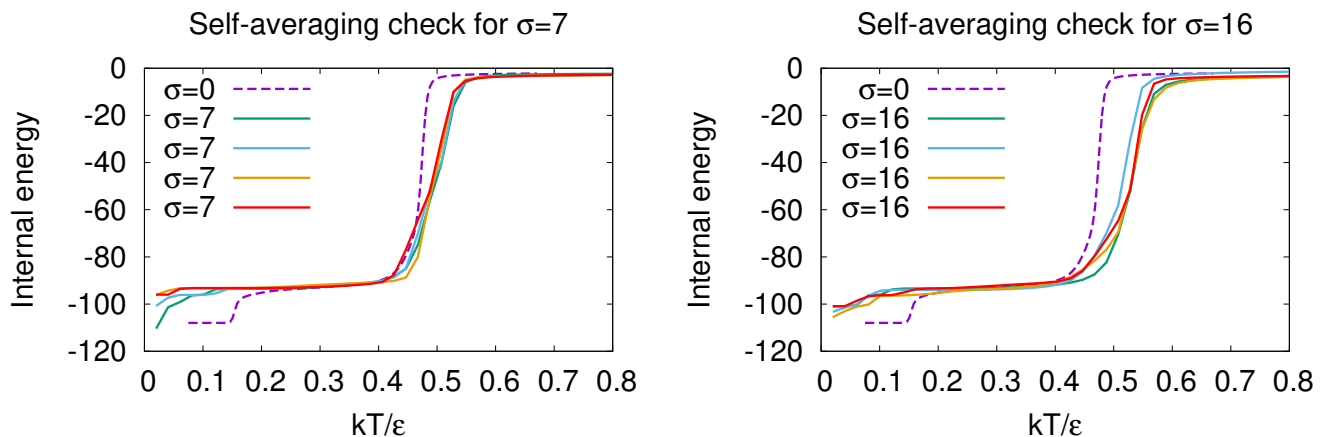


Fig. S2: The curves of internal energy for different realizations are in good agreement with each other for $\sigma = 7, 16$, so we conclude that the internal energy is self-averaging. Four simulations were performed for each of the two values of variance and different realization of the disorder were used in each run (each realization is coded with a different color). These simulations were performed with $N = 257$, $\eta = 17/257$, $R = 0.77$, $\lambda = 1.42$, $1.8 \cdot 10^9$ Monte Carlo sweeps.

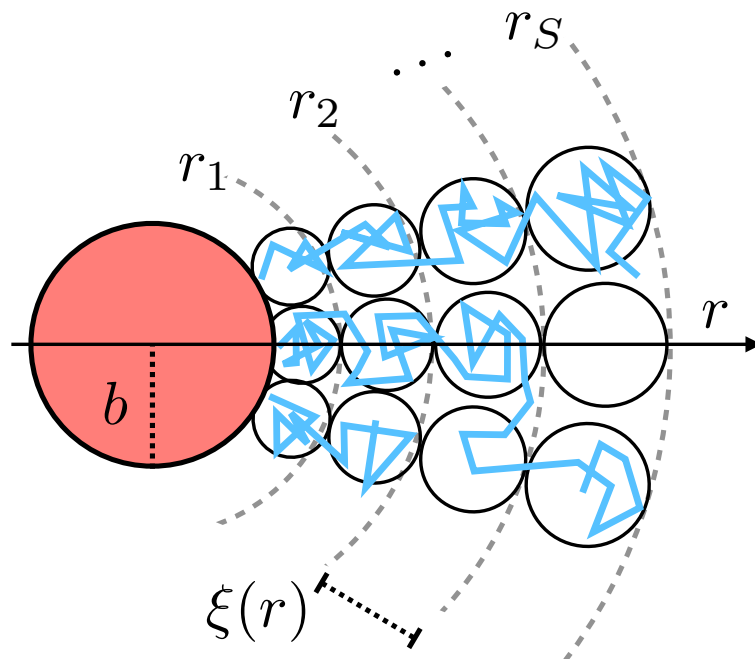


Fig. S3: A single rosette can be approximated by a star polymer, so that it can be described using the blob model. The core of the rosette is described as a rigid sphere of radius b (in red in the sketch), while the loops are approximated as simple polymeric arms (in blue in the sketch) attached to the rigid core. The arms of the star polymer are organized in a series of S concentric shells of thickness $\xi(r)$, which is the size of the blobs at the radial coordinate r .