

Entropy-Based Mechanism of Ribosome-Nucleoid Segregation in *E. coli* Cells

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Supporting Material

Geometrical Considerations of Bond-Beads

Our model represents the contour of DNA plectonemes as single phantom bonds between two terminal beads. These phantom bonds do not exclude any volume to any type of bead. We estimate the volume excluded to ribosomes by the real plectonemic structure as:

$$V_{plectoneme} = \pi(R_{DNA} + R_{ribo})^2(L_{bond}/0.4), \quad (S1)$$

where $R_{DNA} = 1$ nm is the radius of dsDNA, $R_{ribo} = 10$ nm is the radius of the ribosome, $L_{bond} = 200$ nm is the bond length and 0.4 is the ratio of the total plectonemic supercoil contour length to the total DNA double-helix contour length, given the assumed plectoneme geometry. That is, $L_{bond}/0.4$ is the contour length of the two strands of dsDNA between two beads in the plectoneme model. In our coarse-grained model, the volume excluded to ribosomes is:

$$V_{model} = \frac{4}{3}\pi n_{mono}(R_{mono} + R_{ribo})^3, \quad (S2)$$

where $R_{mono} = 10$ nm is the radius of the monomer and n_{mono} is the number of monomers per bond. Solving Eqs. 1 and 2 for n_{mono} yields $n_{mono} = 5.6$. The two node beads at the ends of bond contribute roughly 0.5 beads each to n_{mono} . In practice, we added four additional bond-beads per bond, bringing the value of n_{mono} to 5 for the calculations (Fig. 1C). On the other hand, a similar estimate of the number of monomers per bond required to account for bond-bond excluded volume required on 0.175 beads describing DNA-DNA excluded volume. That is, the volume excluded to a piece of dsDNA by another piece of dsDNA is nearly zero. In order to simultaneously implement these two effects in our simulation, we make the four bond-beads exclude volume for a ribosome but allow mutual overlap between bond-beads. These geometric considerations ignore any configuration or density dependence to the excluded volume, and so are merely estimates of the amount of excluded volume.

Additional Quantification of Equilibrium Distributions

We obtain smooth, equilibrium density distributions by averaging over the snapshots taken throughout a production run, using the cylindrical symmetry of the model to convert the xyz positions into zr positions, where z is the axial coordinate and r the radial coordinate. In Fig. S1, we depict the average number density as a function of position in the cell. This is equivalent to the average density in a thin slab containing the long symmetry axis of the cell. As also observed in the single snapshots, the DNA polymer is highly enriched in the center of the cell and depleted from the periphery. The ribosome distribution is complementary to that of the DNA. The plots in Fig. S1 show the equilibrium DNA bead density vs the axial coordinate z (further averaged over the radial coordinate r at each z). Within a transverse slab of the cell, Fig. S1b shows the equilibrium DNA bead density vs r (averaged over z). The width of the slab is one-half the length of the cylinder region and centered at the midplane. These plots include all the molecules in this slab and are normalized so that the average concentration in this slab is unity. The non-zero concentration near the axis shows that segregation of the DNA polymer from the polysome chains is very strong, but not complete.

TABLE S1: Experimental basis for parameters.

Quantity/symbol		Units	Alanine/poor growth medium	Glucose/moderate growth medium
Doubling time [*]	τ_D	min	150	44
Volume/cell [*]	V_T	μm^3	0.46	1.06
Total cell length [*]	L_{cell}	μm	2.5	3.0
Cell radius [*]	R_{cell}	μm	0.25	0.35
Ribosomes/cell [*]	N_{ribo}	10^3 ribosomes	5	20
Distance of ribosomes on mRNA [†]	R_m/N_r	nucleotides/ ribosome	90	68
Specific linking deficit [‡]	σ_{link}		0.03	0.03
Plectoneme opening angle [§]	α	degrees	56.2	56.2
Plectoneme radius [§]	r	nm	11.8	11.8
Persistence length of plectoneme [¶]	l_p	nm	83	83
DNA/cell [*]	G_C	genome equivalents	1.2	2.1
DNA/cell	G_C (bp)	10^6 bp	5.52	9.66
DNA/cell [§]	L_{DNA}	10^6 nm	1.88	3.28
DNA/cell ^{**}	$L_{plectoneme}$	10^6 nm	0.78	1.36

* Taken from table 1 in (S1). Very similar values can be found in (S2).

† Data from table 3 in (S2) extrapolated and interpolated to growth rates of 150 and 44 minutes respectively.

‡ From an estimate of 0.06 as the total specific linking deficit and that roughly 50% is compensated for by DNA binding proteins (S3).

§ From table 6 in (S4). See similar results in (S5).

¶ $l_p = 2p \sin(\alpha)$ with $p=50$ nm, the persistence length for dsDNA in high salt (S6).

|| Based on G_C and 4.6 Mbp, the length of the *E. coli* MG1655 genome (S7).

§ Assuming 0.34 nm/bp for DNA.

$$** L_{plectoneme} \approx \frac{L_{DNA} \sin \alpha}{2}.$$

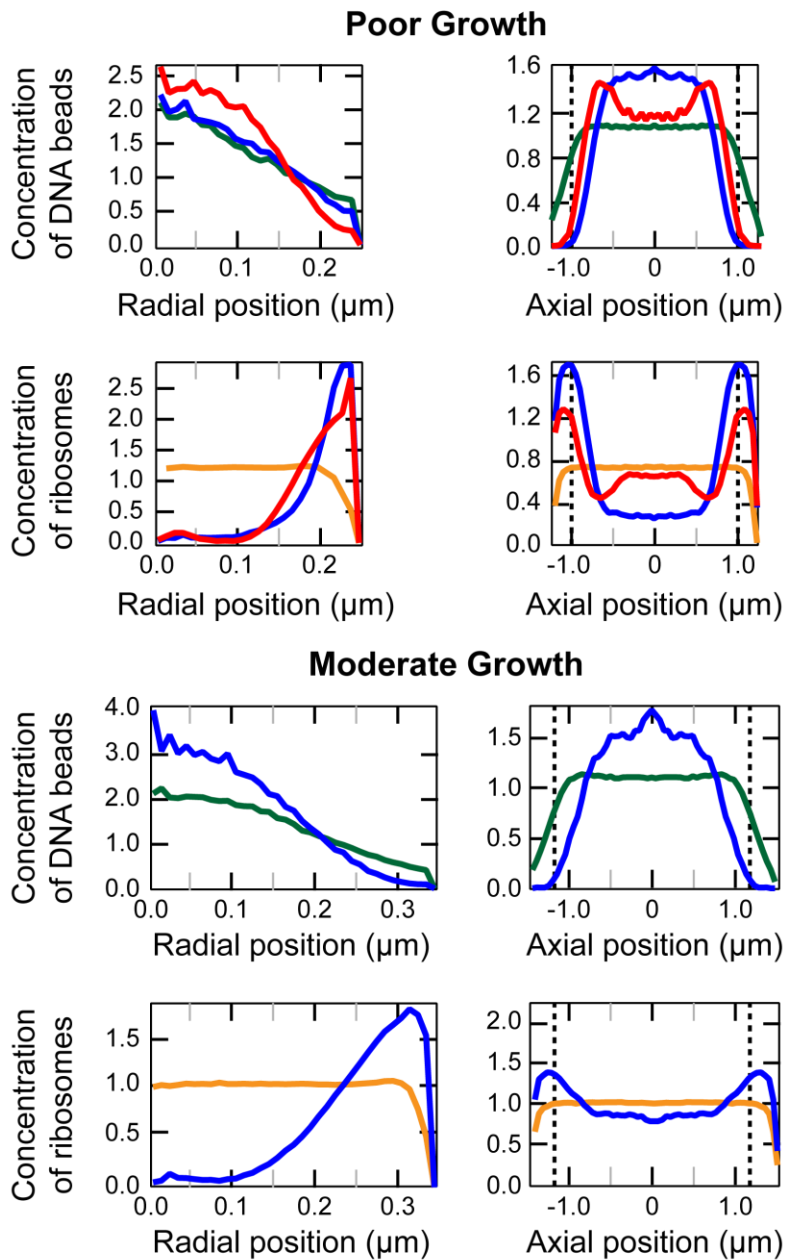


Figure S1. Equilibrium distribution of DNA and ribosome beads measured as the mean concentration in a thin, central slab containing the long axis of the cell. Radial coordinate is r , axial coordinate is z . Axial plots average over all r for a given z and are normalized so that the average concentration in the entire cell is unity. The radial plots average only over a central rectangular slab whose width is half the cylindrical region's length. The radial plots are normalized so that the average concentration in this slab is unity. The color of each plot corresponds to the model type: ribosomes only (orange), DNA only (green), DNA and polysomes (blue), and DNA and ribosome monomers (red). The dotted lines in the axial profiles indicate the end of the cylindrical regions in the model.

Supporting references

- S1. Woldringh, C. L., and N. Nanninga. 1985. Structure of nucleoid and cytoplasm in the intact cell. In *Molecular cytology of Escherichia coli*. N. Nanninga, editor. Academic Press, London. 161-197.
- S2. Bremer, H., and P. P. Dennis. 1996. Modulation of chemical composition and other parameters of the cell by growth rate. In *Escherichia coli and Salmonella: Cellular and molecular biology*. ASM Press, Washington, D.C. 1553-1569.
- S3. Charlebois, R. 1999. Organization of the prokaryotic genome. ASM Press, Washington D.C.
- S4. Ubbink, J., and T. Odijk. 1999. Electrostatic-undulatory theory of plectonemically supercoiled DNA. *Biophysical Journal* 76:2502-2519.
- S5. Boles, T. C., J. H. White, and N. R. Cozzarelli. 1990. Structure of plectonemically supercoiled DNA. *Journal of Molecular Biology* 213:931-951.
- S6. Cunha, S., C. L. Woldringh, and T. Odijk. 2001. Polymer-mediated compaction and internal dynamics of isolated *Escherichia coli* nucleoids. *Journal of Structural Biology* 136:53-66.
- S7. Blattner, F. R., G. Plunkett, C. A. Bloch, N. T. Perna, V. Burland, M. Riley, J. Collado-Vides, J. D. Glasner, C. K. Rode, G. F. Mayhew, J. Gregor, N. W. Davis, H. A. Kirkpatrick, M. A. Goeden, D. J. Rose, B. Mau, and Y. Shao. 1997. The complete genome sequence of *Escherichia coli* K-12. *Science* 277:1453-1462.