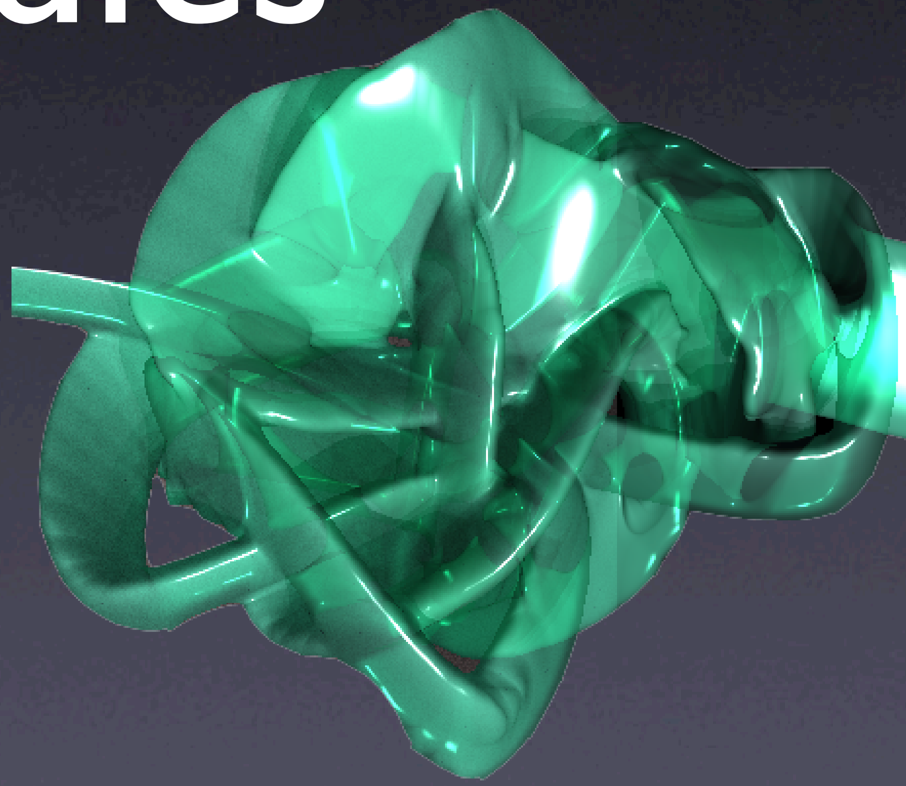
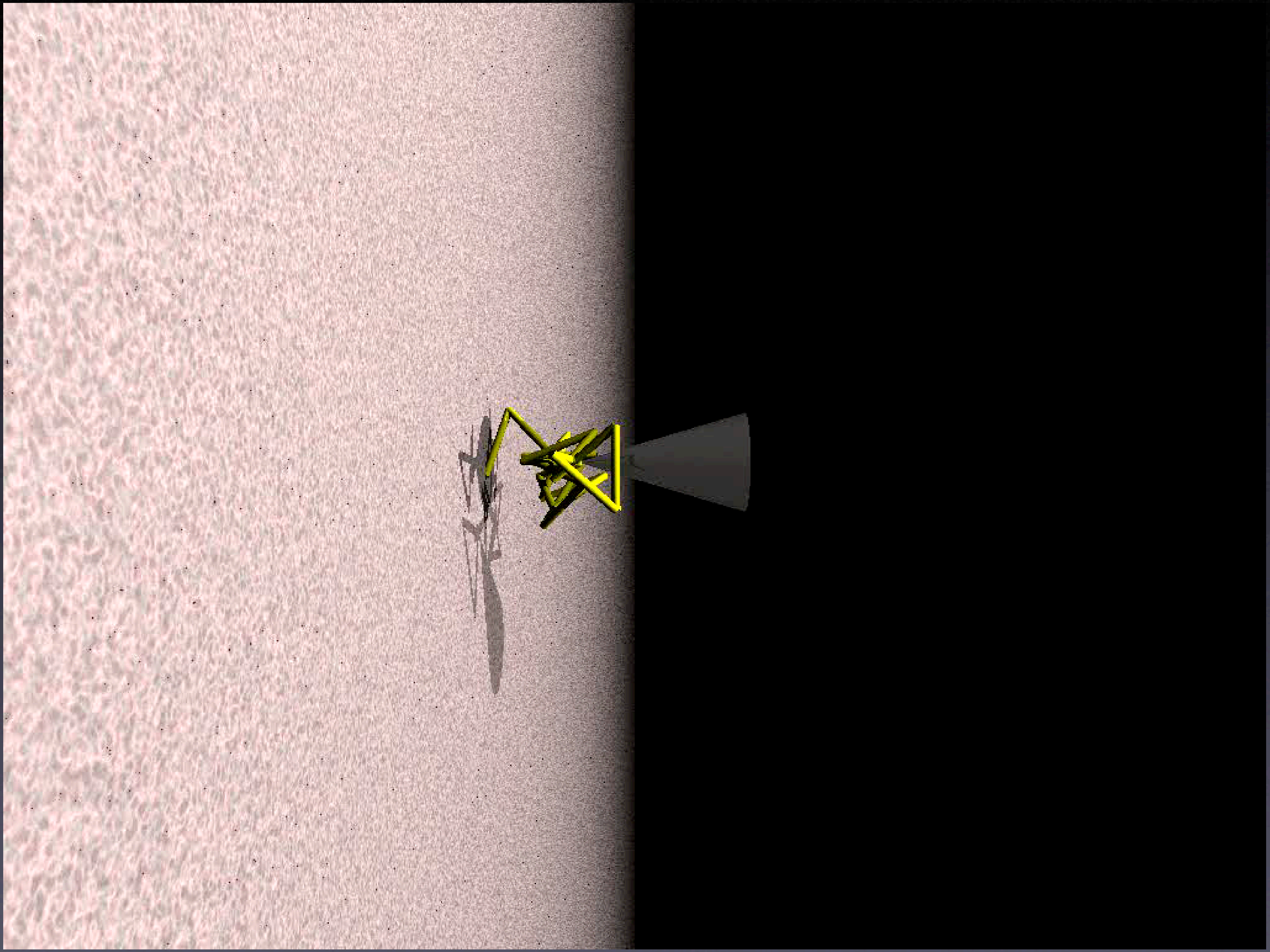
Knots in Macromolecules



Dieter W. Heermann

Heidelberg University 2005

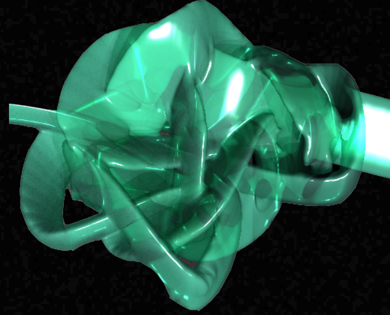
Introduction



Introduction

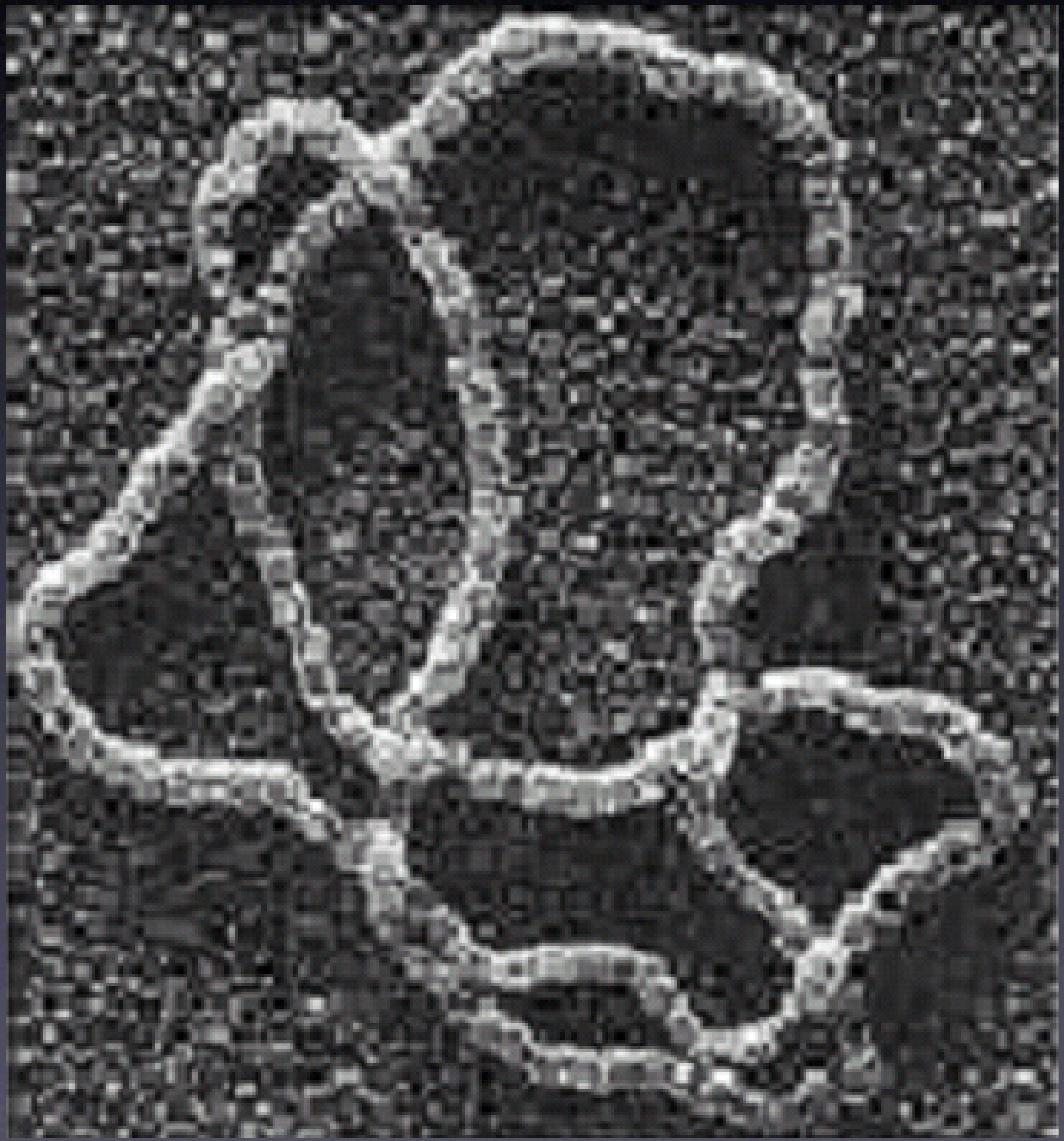
- DNA packing can be visualized as two very long strands that have been intertwined millions of times, tied into knots, and subjected to successive coiling.
- Replication and transcription are much easier to accomplish if the DNA is neatly arranged rather than tangled up in knots.
- Enzymes are essential to unpacking DNA.
- Enzymes act to slice through individual knots and reconnect strands in a more orderly way.

Taken from http://www.smoothbrothers.com/design/design_3d.htm



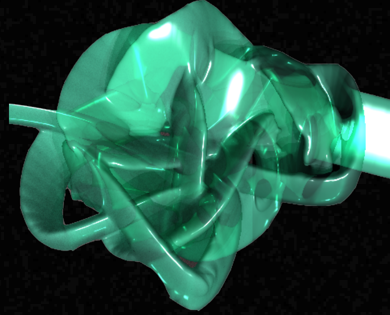
Introduction

- How can knot theory help us understand DNA packing?
- How can we estimate the rates at which enzymes unknot DNA?

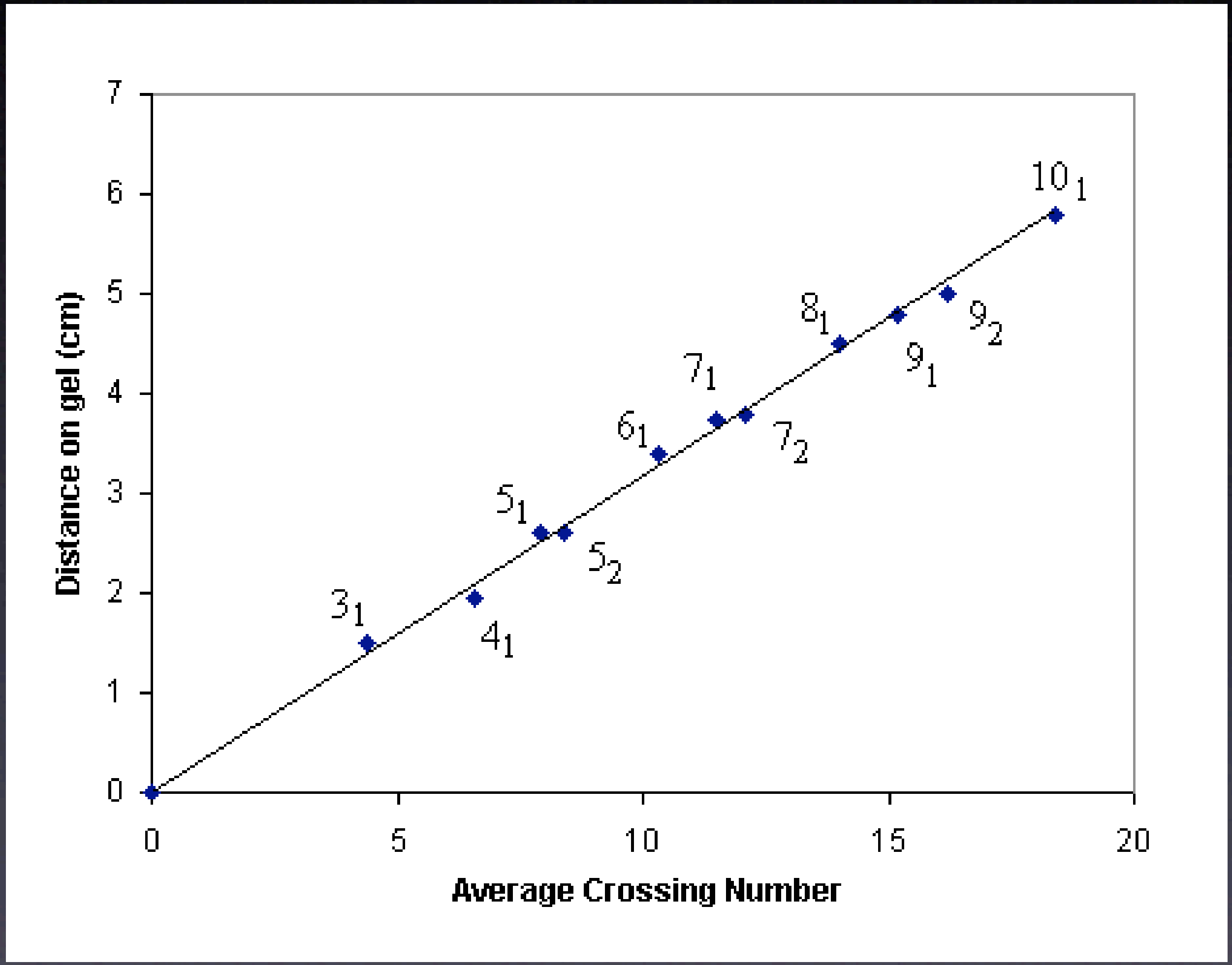


Picture taken from Sumners, D. 1995. Lifting the curtain: Using topology to probe the hidden action of enzymes. Notices of the AMS 42:528-537.

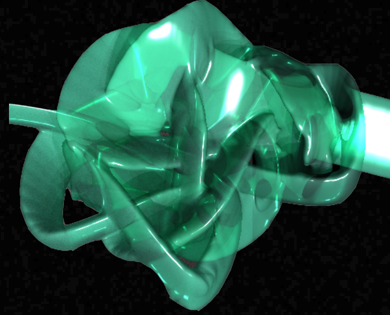
Introduction



- Determining the crossing number of DNA knots involves using gel electrophoresis.
- The distance DNA fragments move on an electrophoretic gel is highly correlated with the average crossing number.



Content



- Average Crossing Number

  Key questions:

  Predict behaviour for chains with excluded volume.

  Distinguish between ln N and a power law.

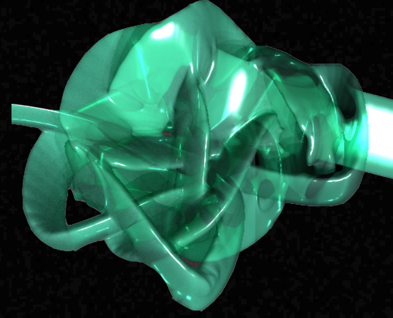
- Statistics of knots

  Key questions:

  Distribution of knots.

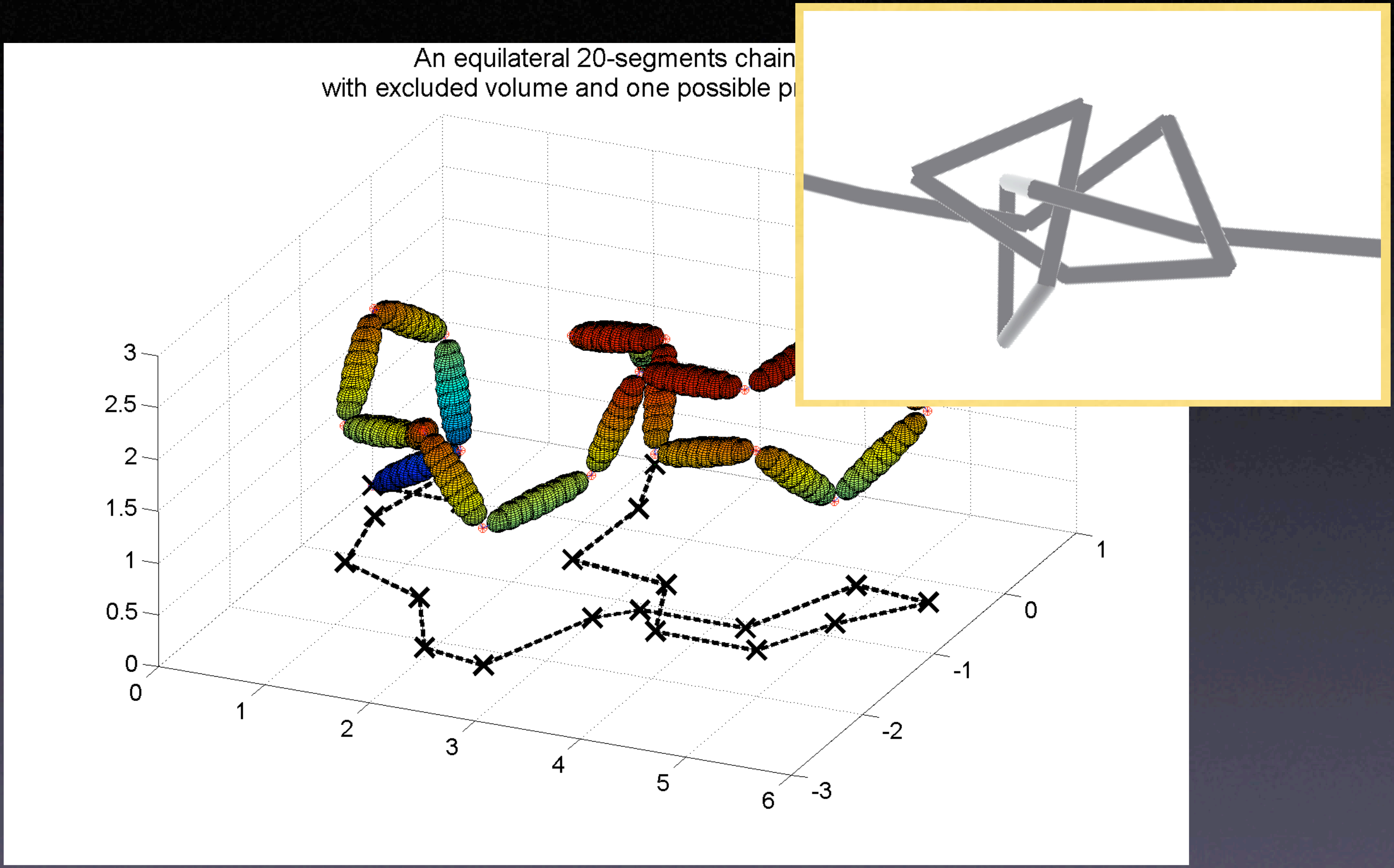
  Average number of monomers in a knot.

Average Crossing Number

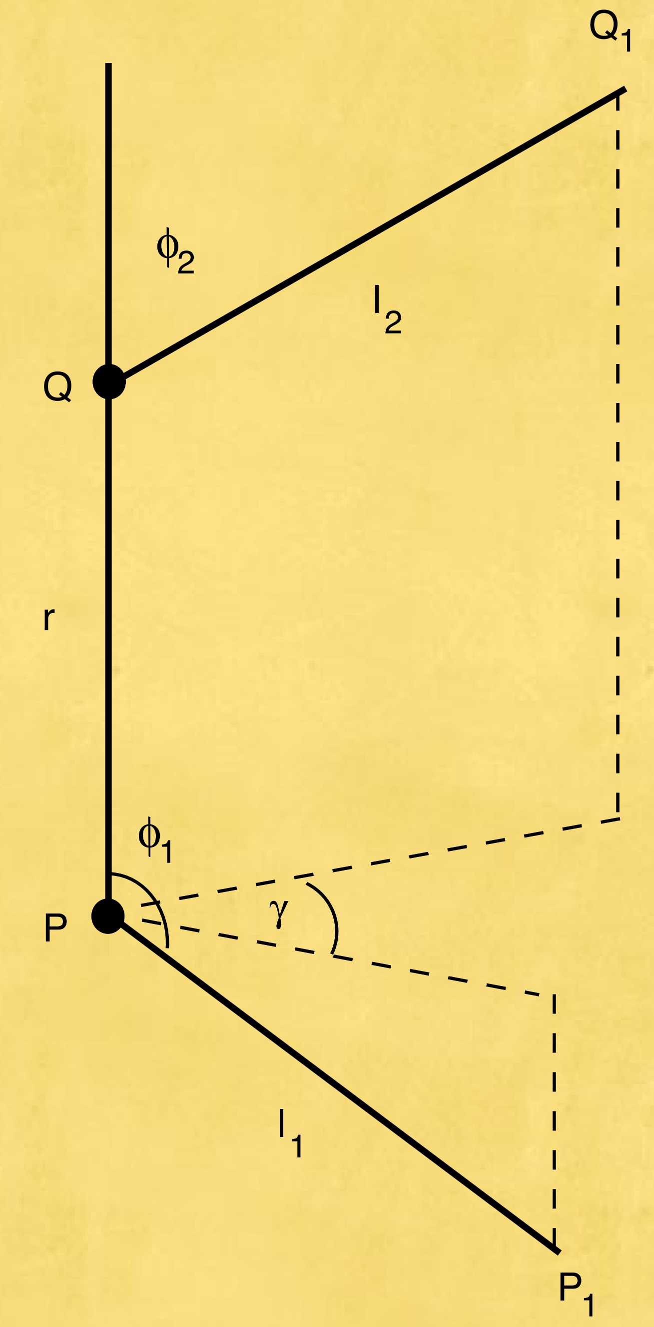


- Investigate the effects of excluded volume interactions on the average crossing number (ACN)
- Look at two kinds of chains:
  - Equilateral and
  - Gaussian random walks

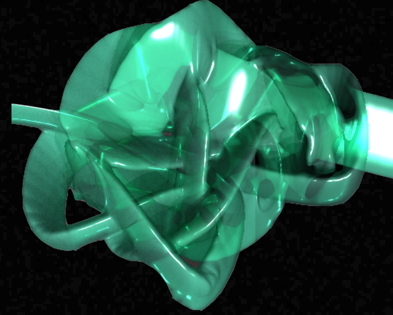
Average Crossing Number



Average Crossing Number



Average Crossing Number



$$a(l_1, l_2) = \frac{1}{2\pi} \int_{\gamma_1} \int_{\gamma_2} \frac{|\dot{\gamma}_1(t), \dot{\gamma}_2(s), \gamma_1(t) - \gamma_2(s)|}{\|\gamma_1(t) - \gamma_2(s)\|^3} \, dt \, ds$$

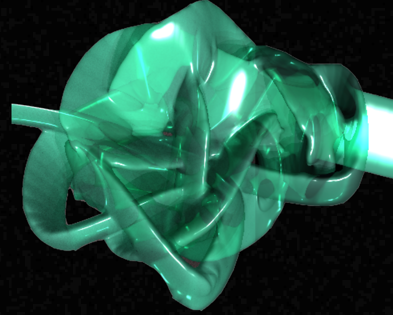
For Gaussian phantom chains

$$< a(l_1, l_2) > \quad = \frac{1}{2\pi d^2} + O\left(\frac{1}{d^{2.5}}\right)$$

For equilateral phantom chains

$$< a(l_1, l_2) > \quad = \frac{1}{16 d^2} + O\left(\frac{1}{d^3}\right)$$

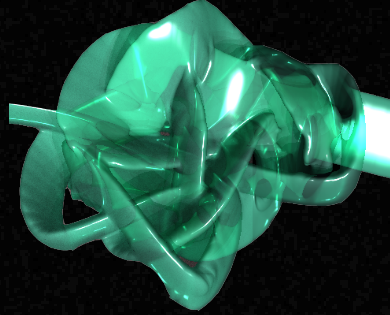
Average Crossing Number

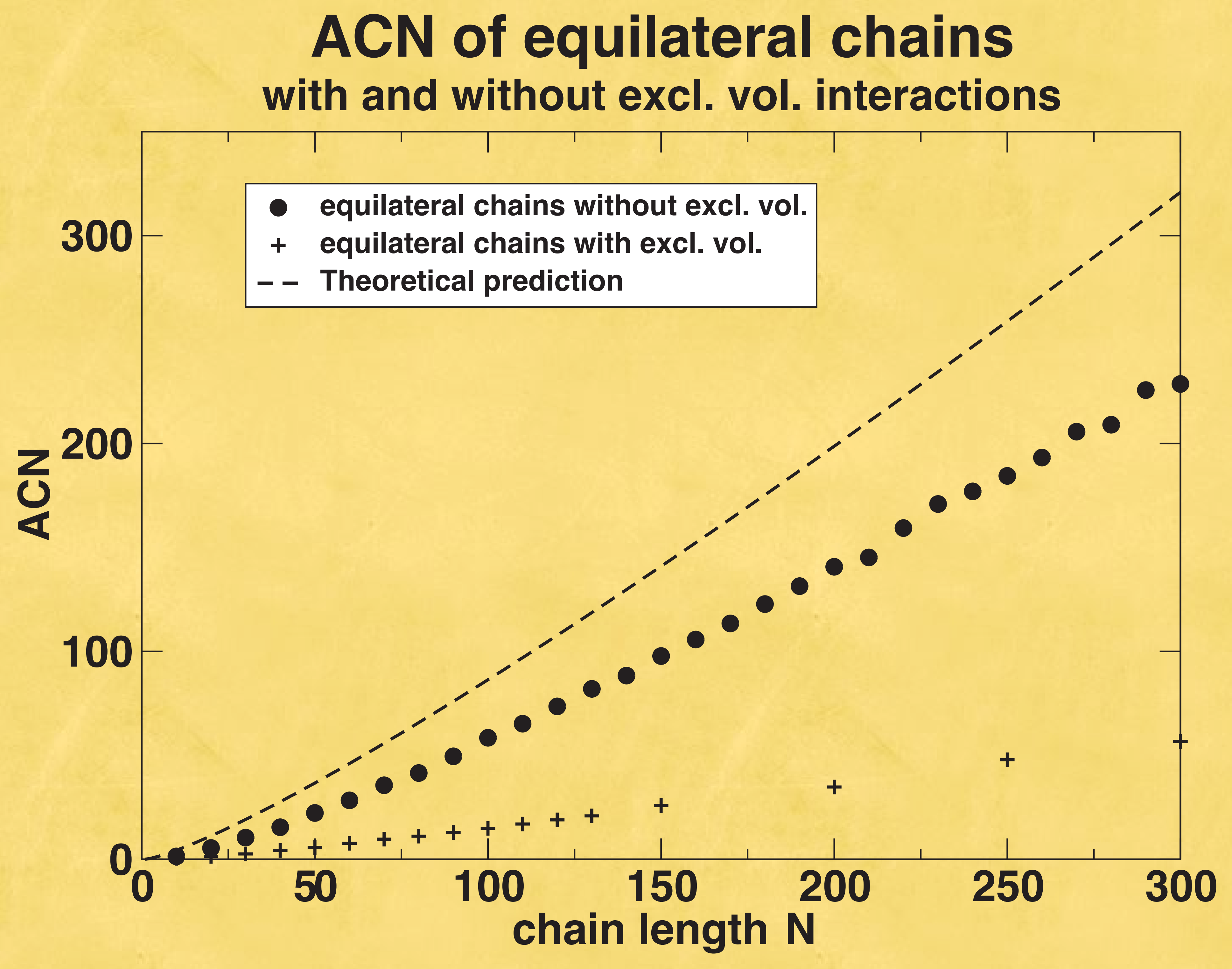


$$
\begin{aligned}
\mathrm{ACN}_{\mathrm{Gaussian}}(N) &= \boxed{\frac{1}{2\pi}} N\, log(N) + O(N) \\
&\approx \frac{1}{2\pi} N\, log(N) + c_1 \cdot N
\end{aligned}
$$

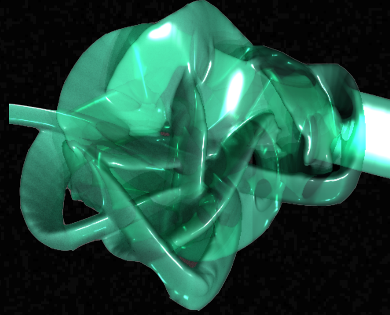
$$
\begin{aligned}
\mathrm{ACN}_{\mathrm{Equilateral}}(N) &= \boxed{\frac{3}{16}} N\, log(N) + O(N) \\
&\approx \frac{3}{16} N\, log(N) + c_2 \cdot N
\end{aligned}
$$

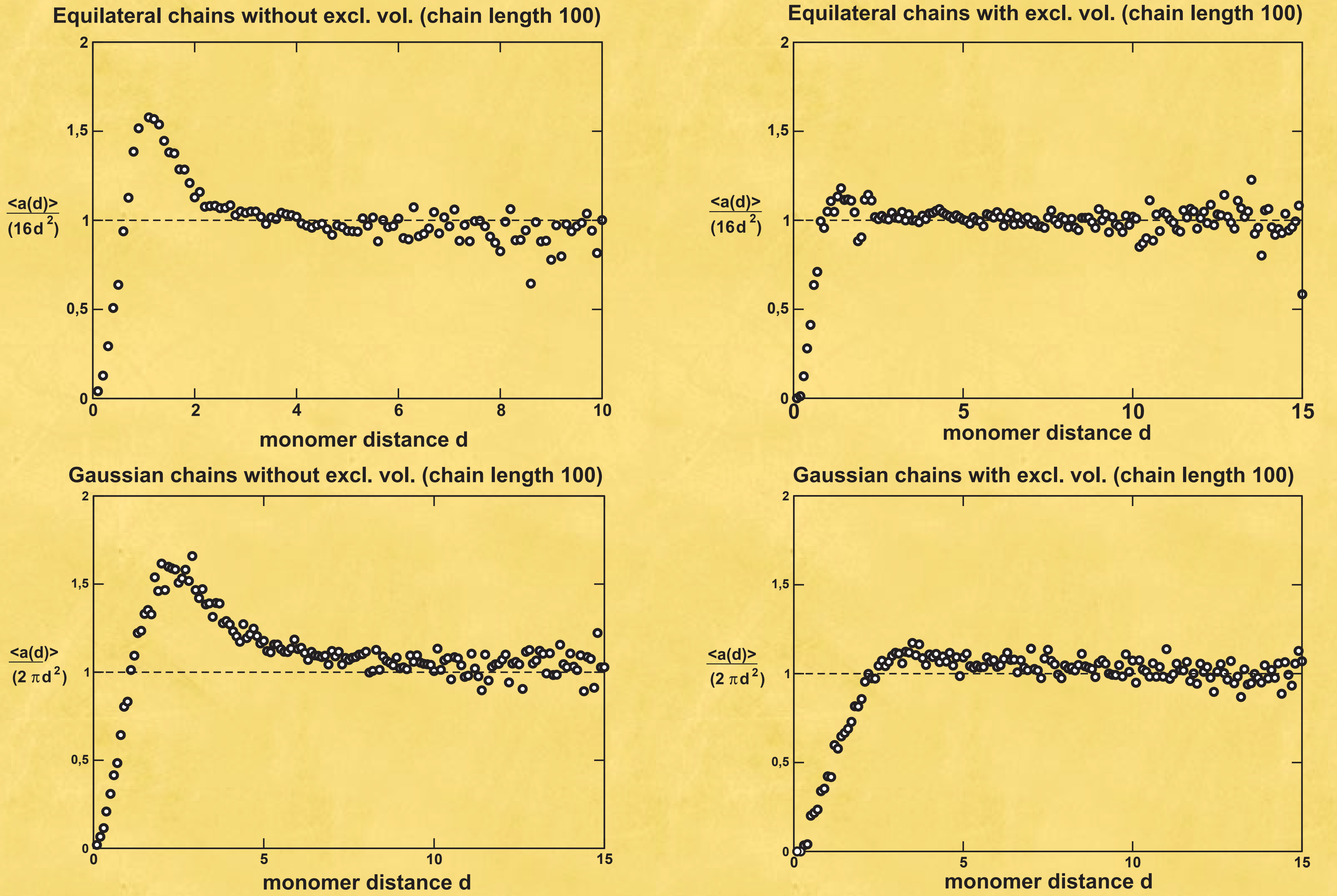
Average Crossing Number





Average Crossing Number





Ratio of simulation results with the leading term from the theoretical prediction

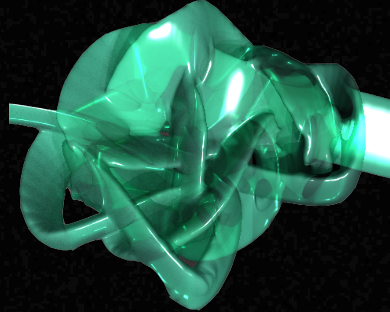
Equilateral chains without excl. vol. (chain length 100)

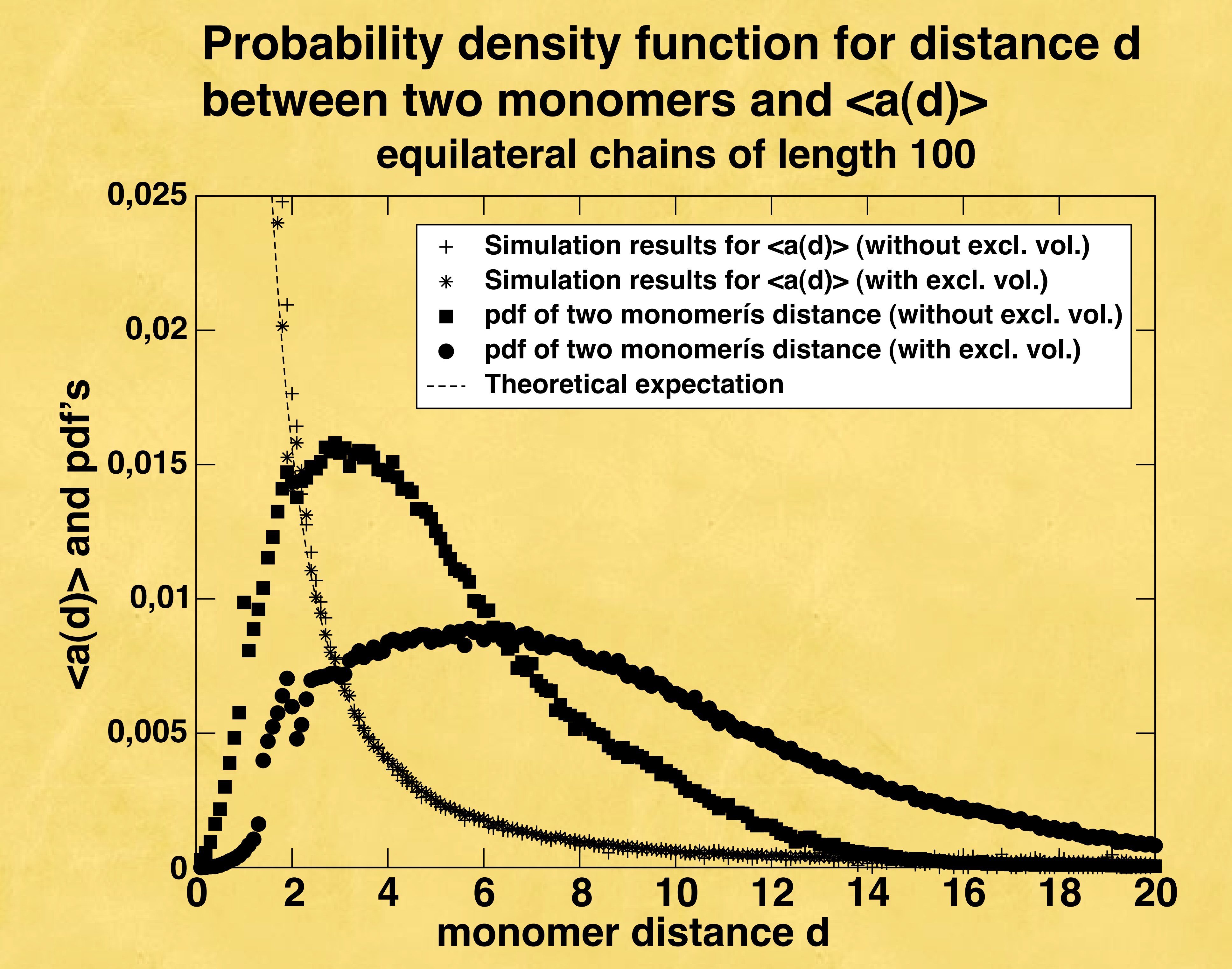
Equilateral chains with excl. vol. (chain length 100)

Gaussian chains without excl. vol. (chain length 100)

Gaussian chains with excl. vol. (chain length 100)

Average Crossing Number





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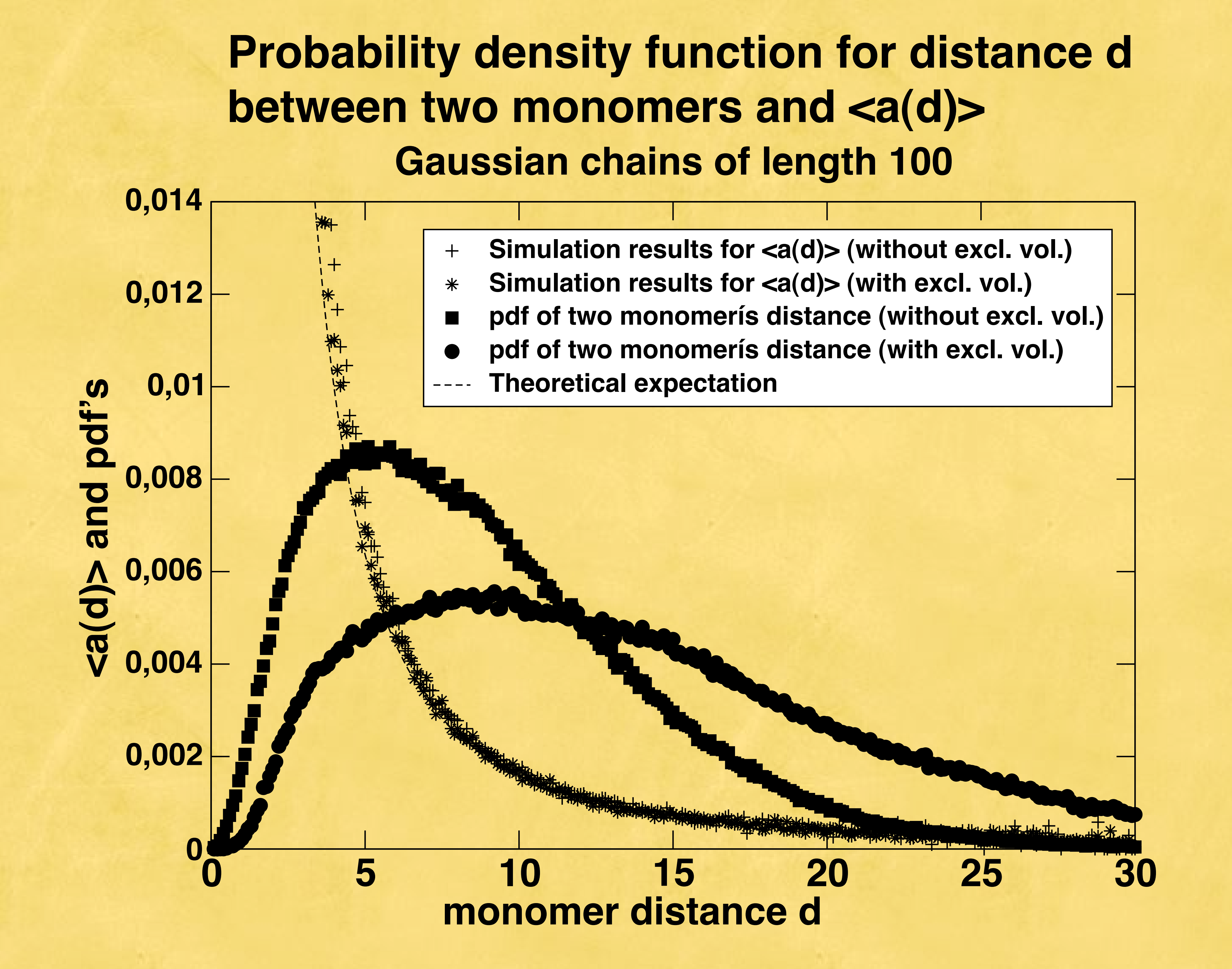

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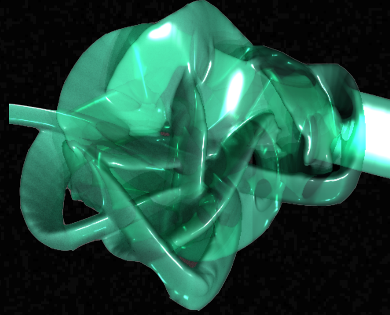

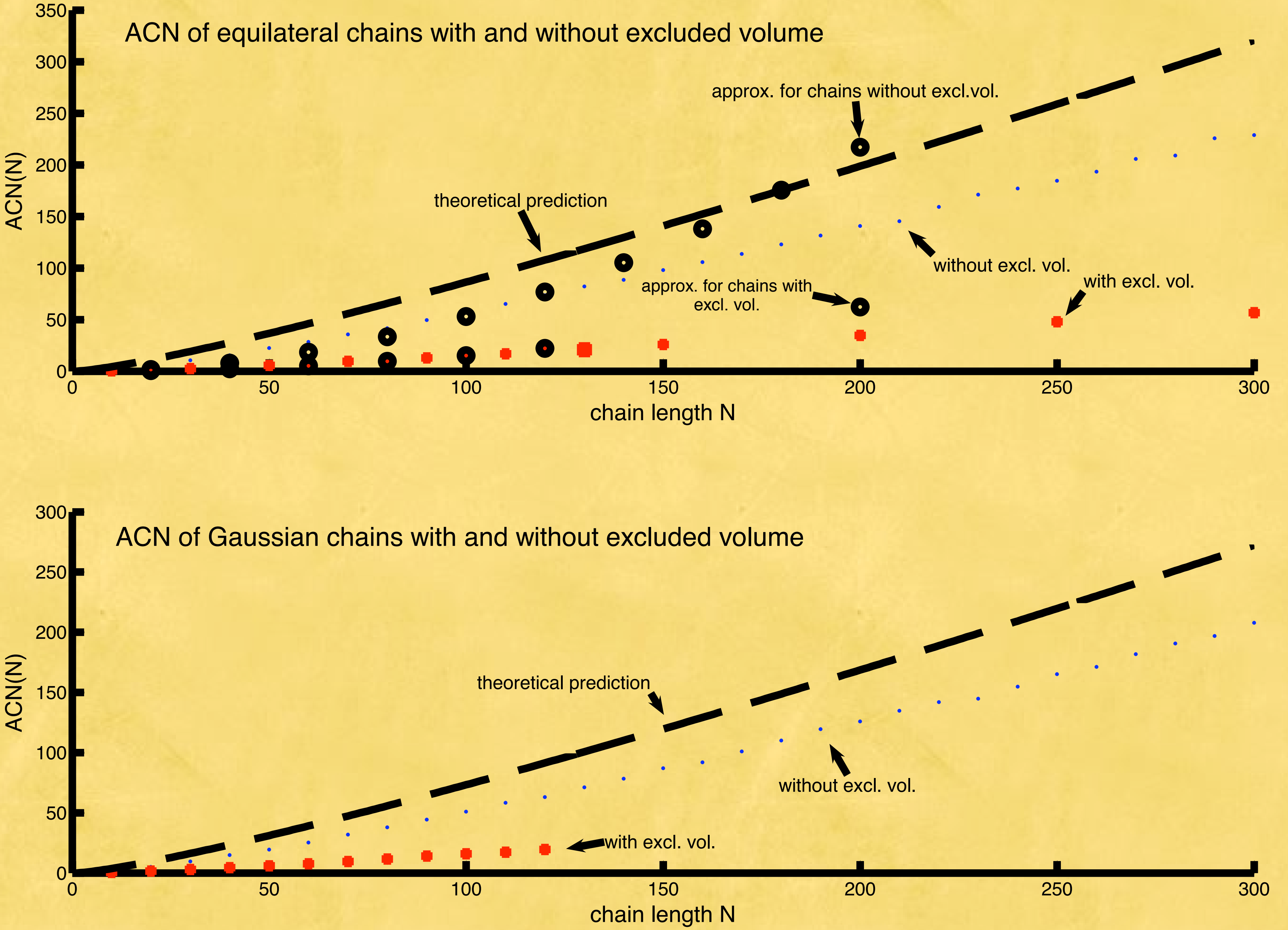

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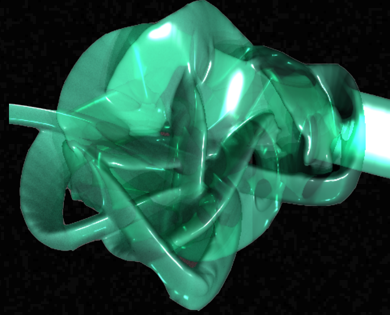

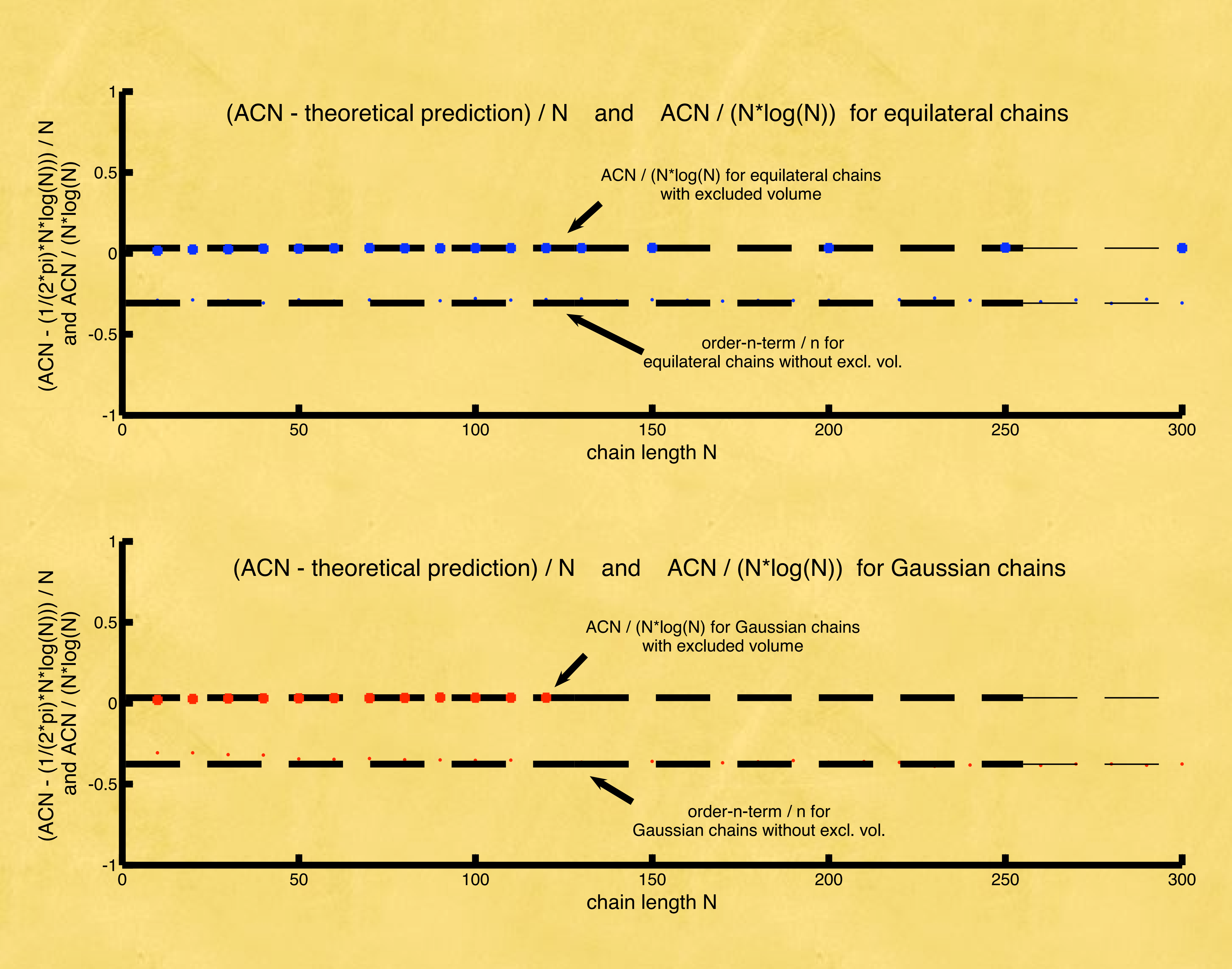

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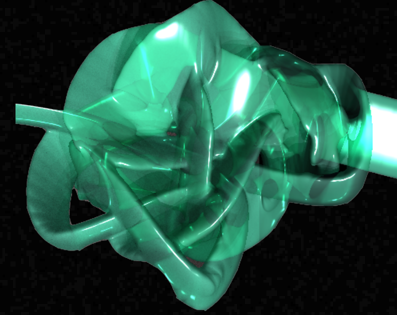
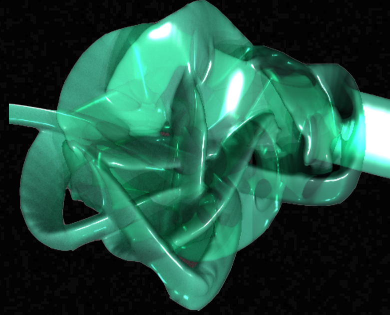


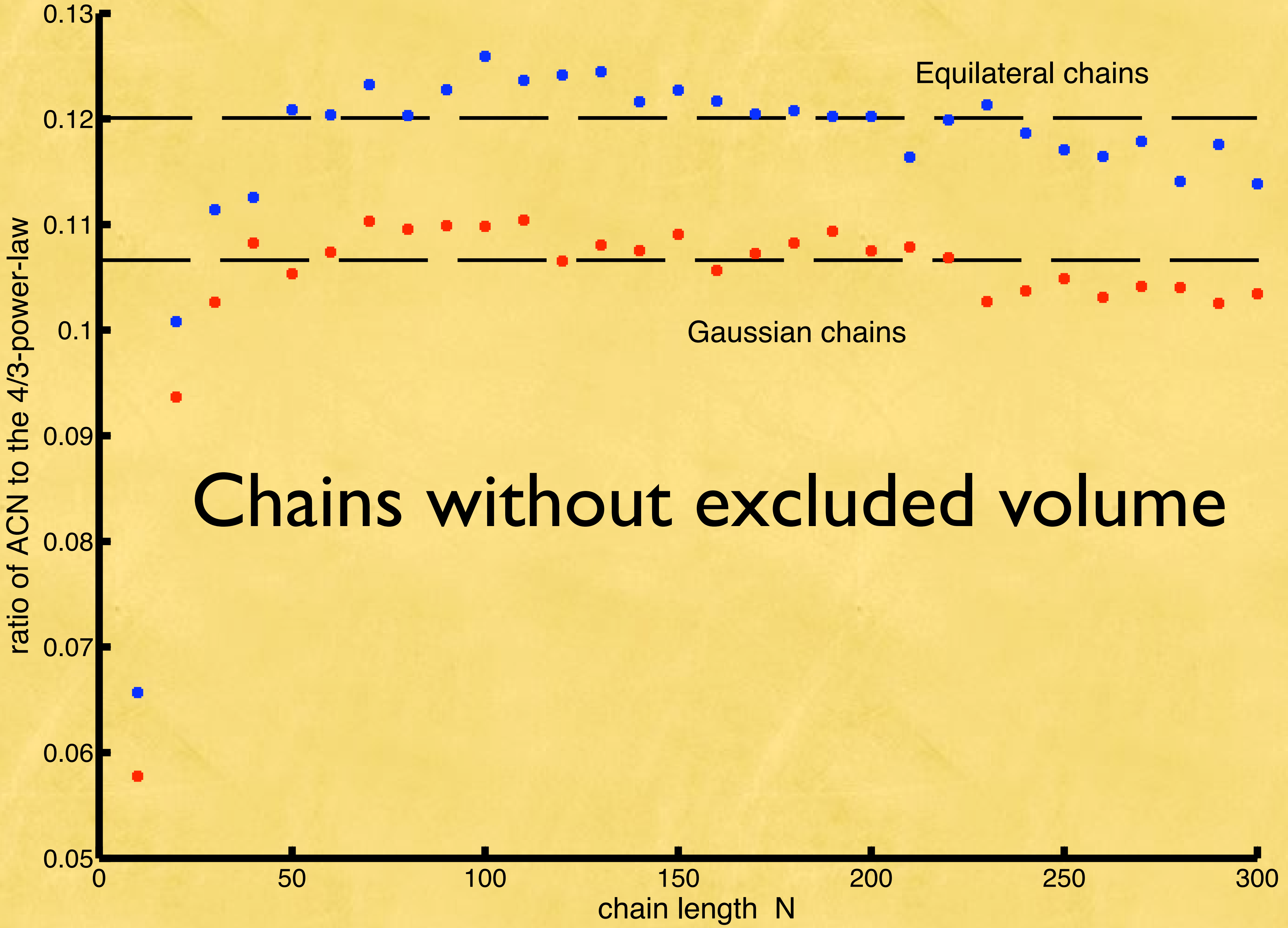
$$N \ln N + c \cdot N$$

$$vs.$$

$$N^{4/3}$$

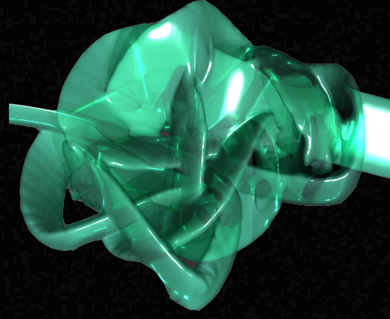
Average Crossing Number

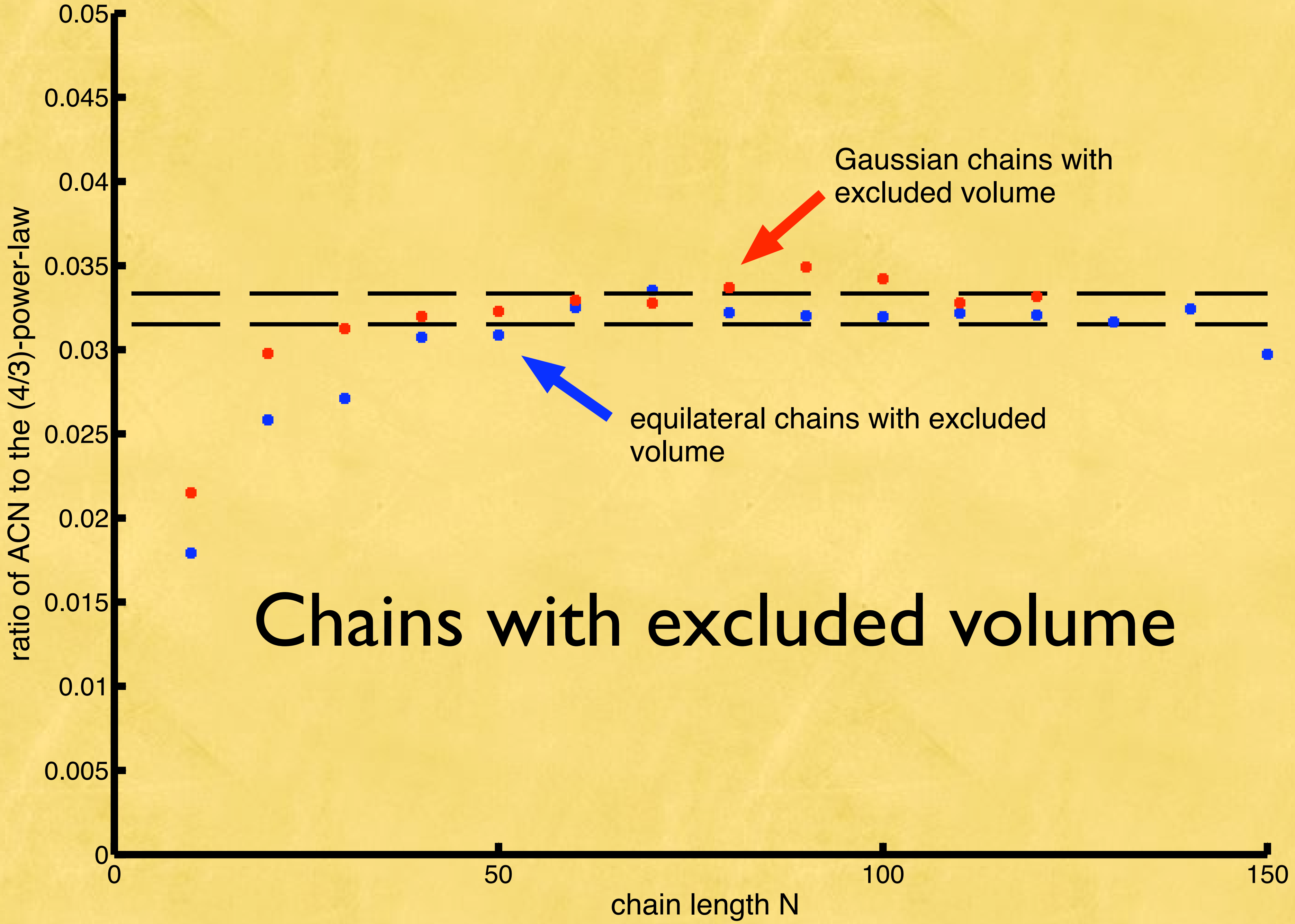




Chains without excluded volume

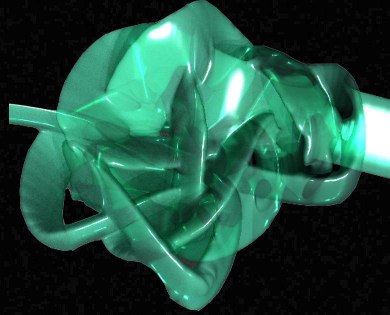
Average Crossing Number



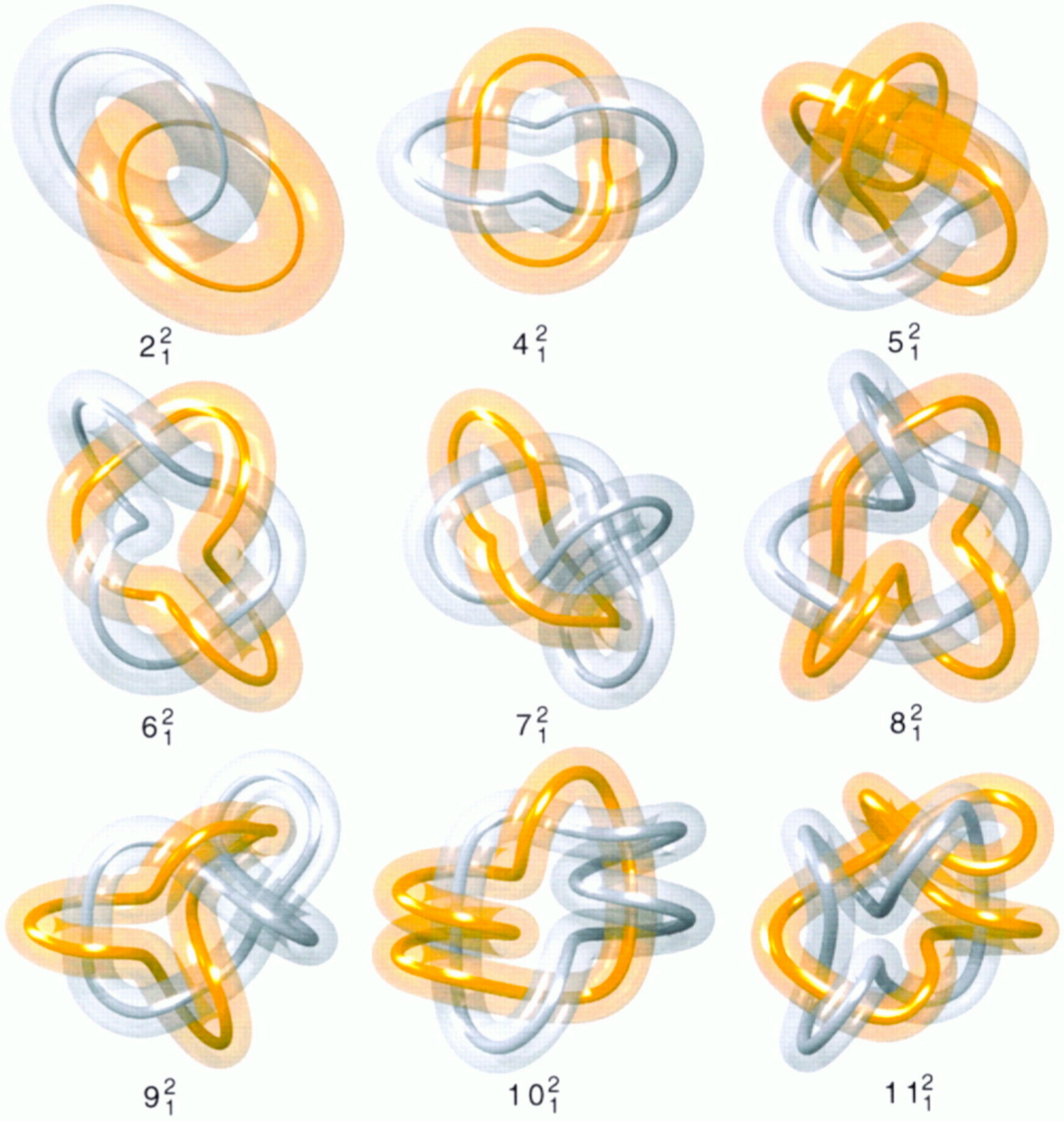


Chains with excluded volume

Statistics of Knots

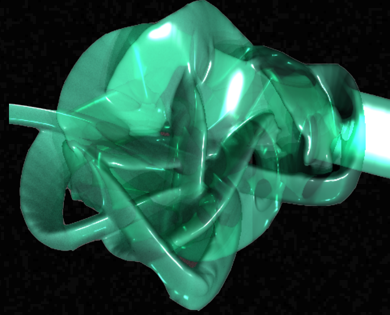


- Topological characterization of knots.
- Alexander, HOMFLY, ... Polynomials
- Here not interested; Chains are open.



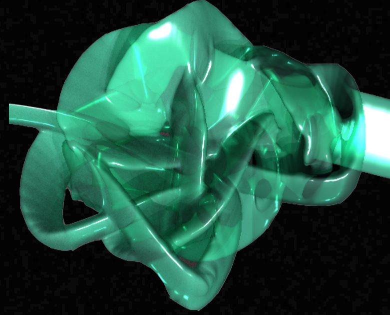
Taken from Geometry and Physics of Catenanes Applied to the Study of DNA Replication
Ben Laurie, Vsevolod Katritch, Jose Sogo, Theo Koller, Jacques Dubochet, and Andrzej Stasiak

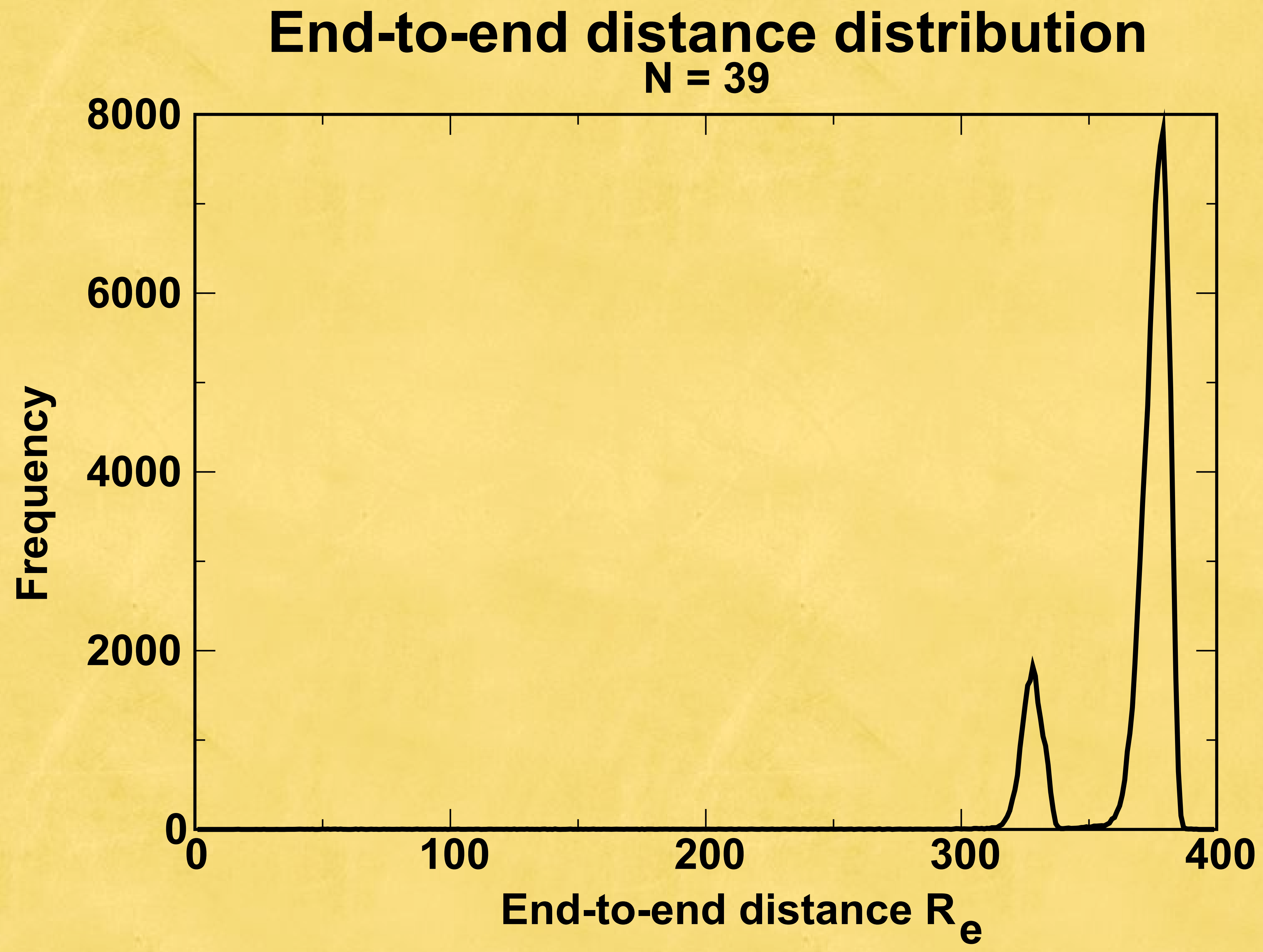
Statistics of Knots



- Here we apply a heuristic approach to the identification of a knot.
- We employ the notion of polymers with entanglement which cannot be reduced to a straight polymer chain.
- Knots are an effect of the self-avoiding property of the macromolecules and they do only occur when we stretch the chain.
- Frisch-Wasserman-Delbrück conjecture

Statistics of Knots





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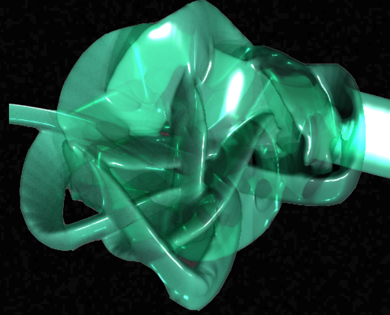

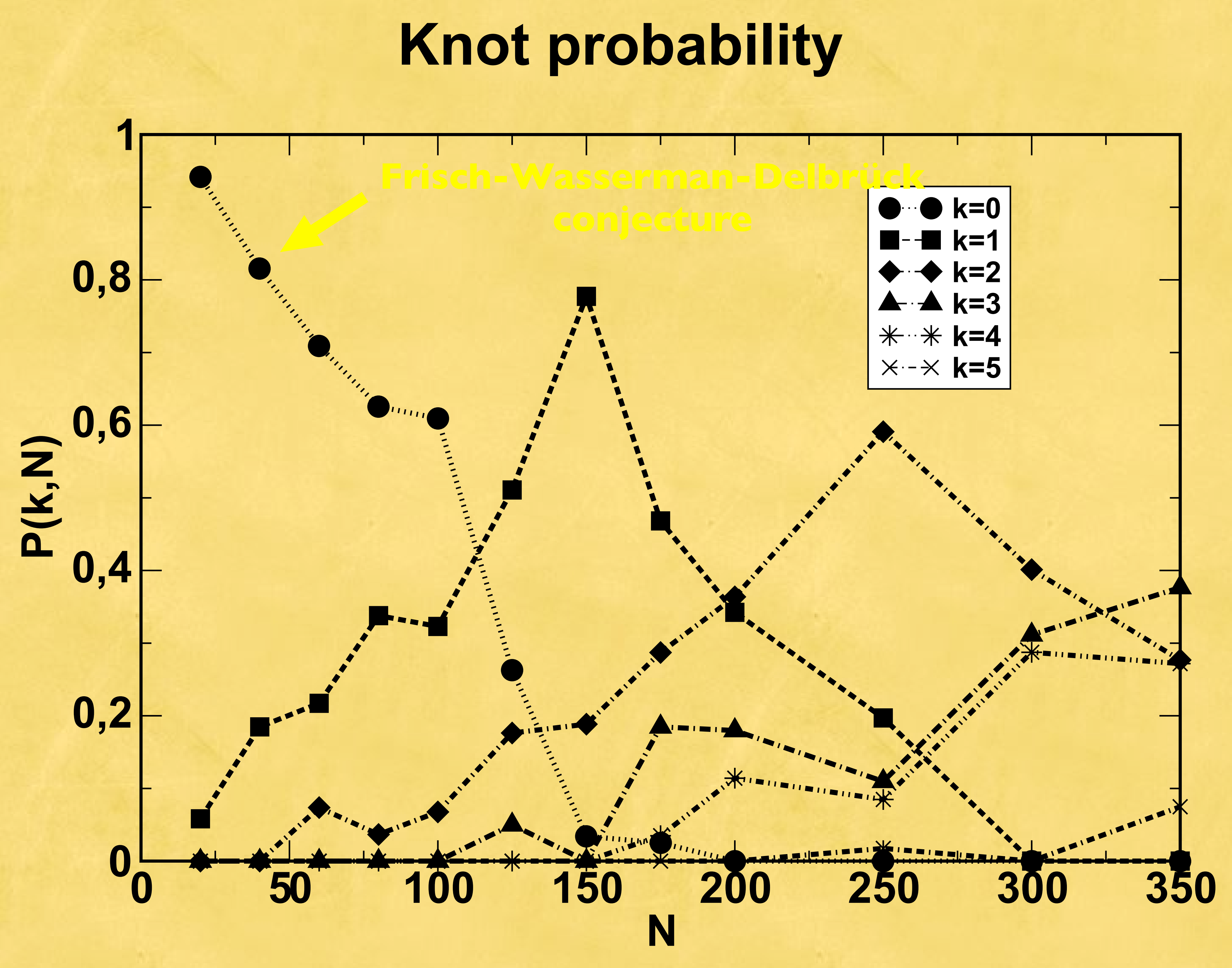

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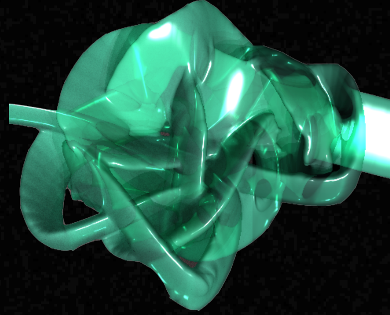
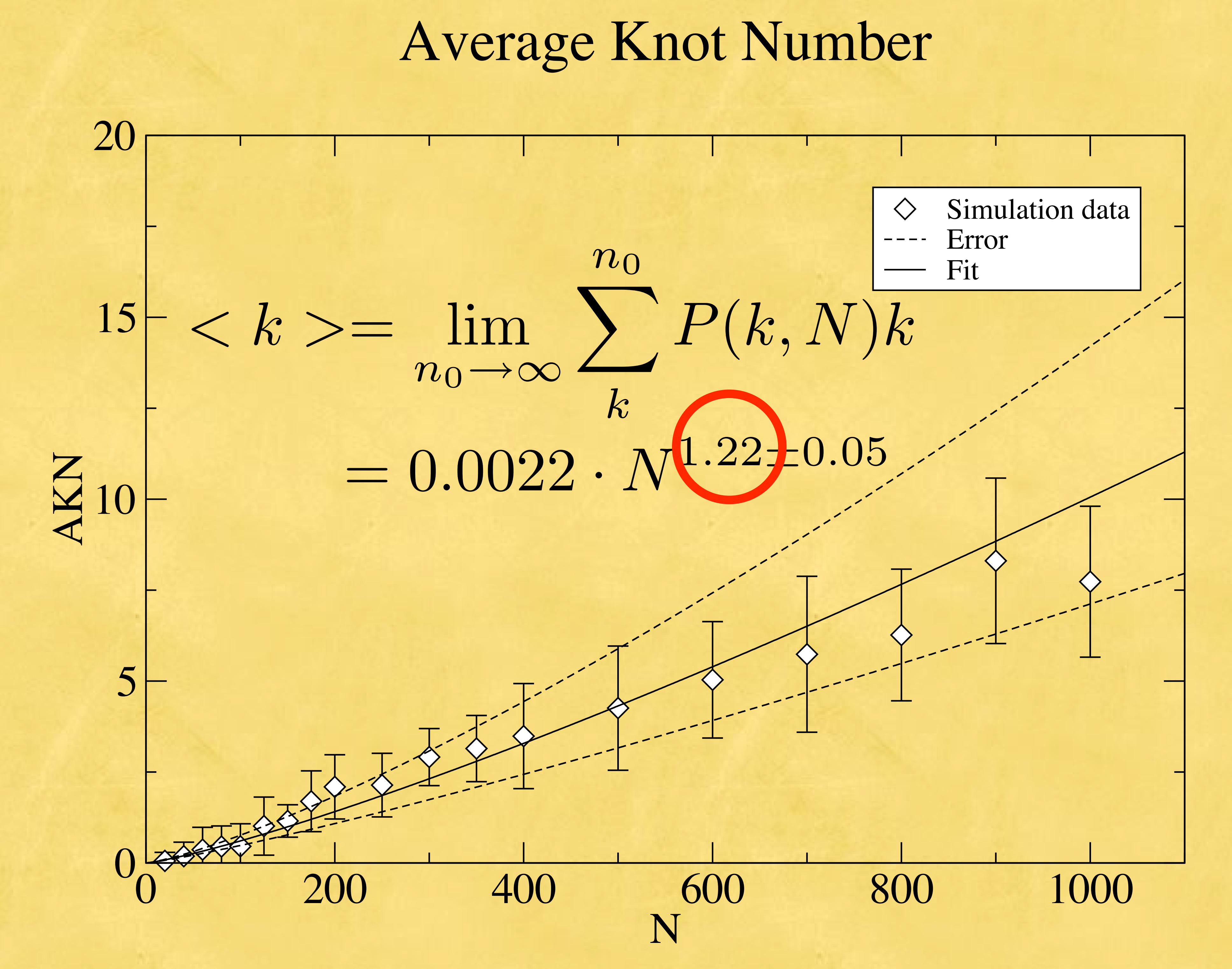
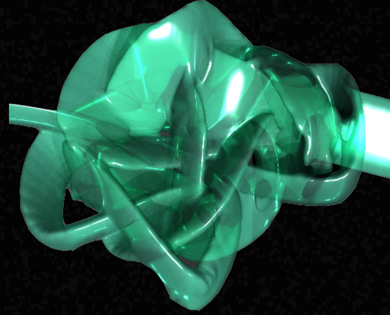


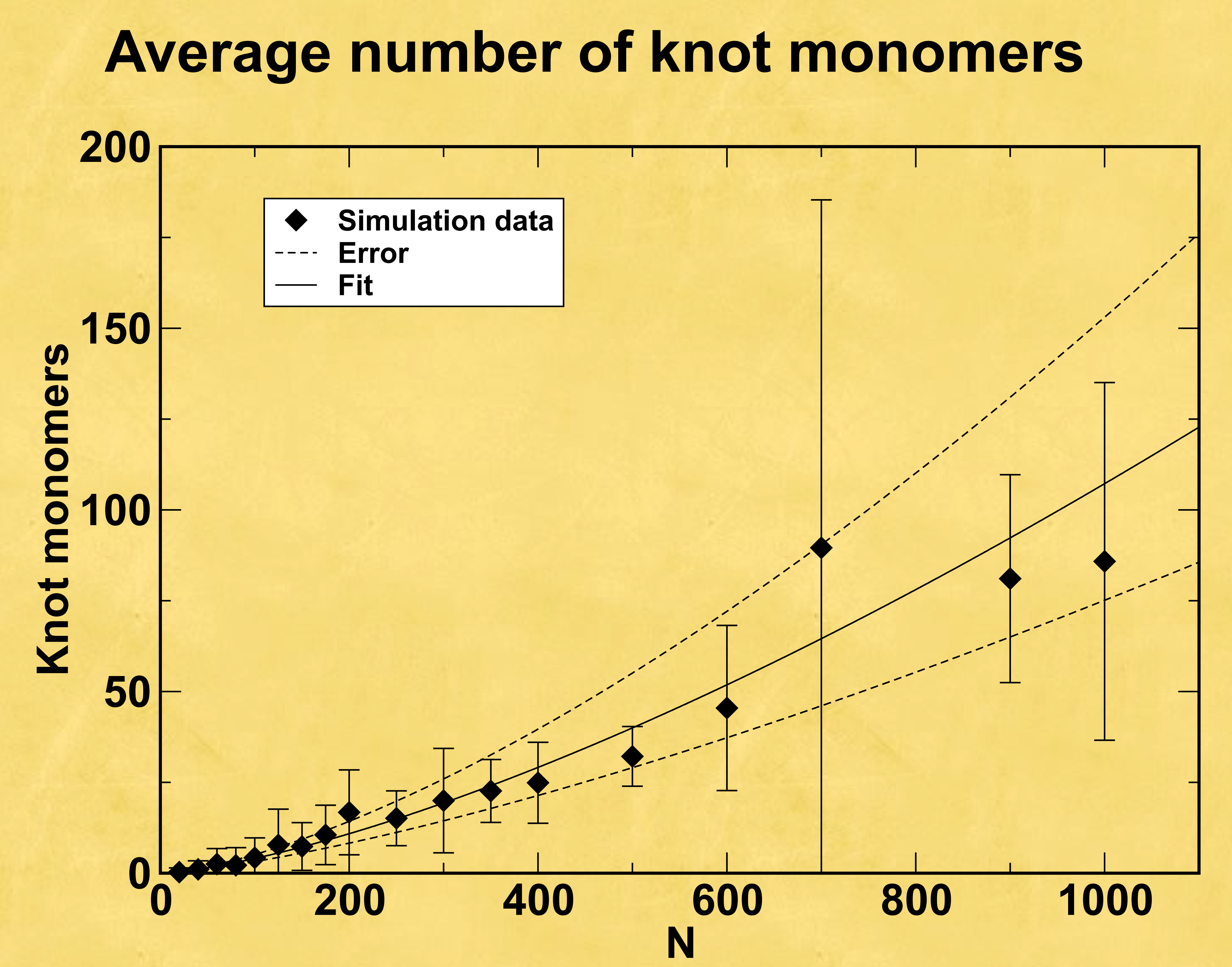


$$< k > = \lim_{n_0 \to \infty} \sum_{k}^{n_0} P(k, N) k$$

$$= 0.0022 \cdot N^{1.22 \pm 0.05}$$

Statistics of Knots





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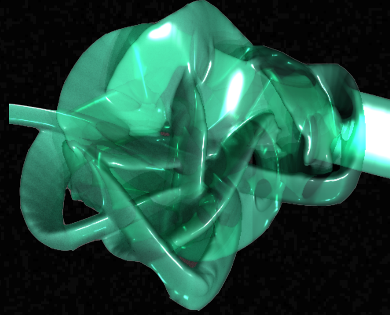

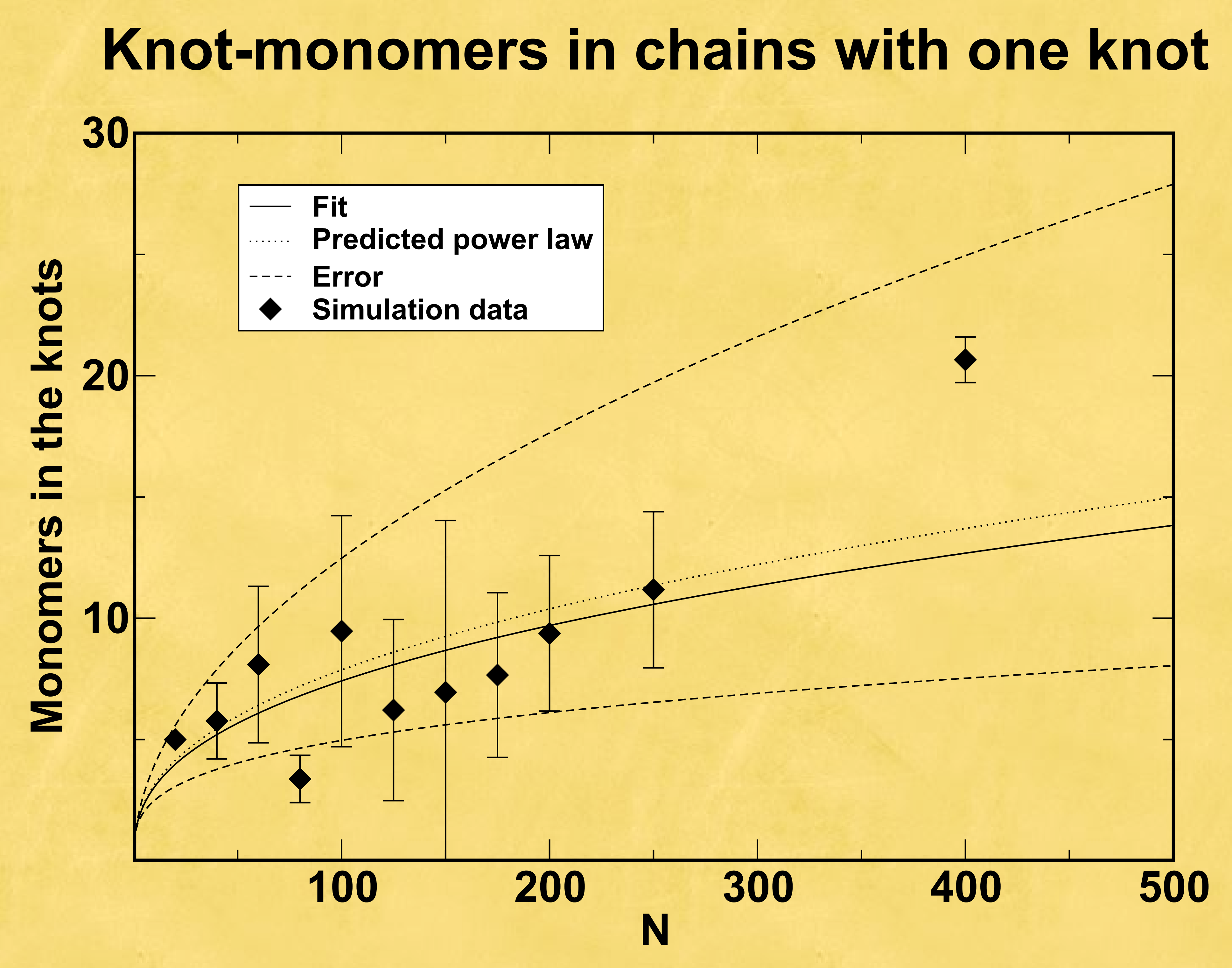

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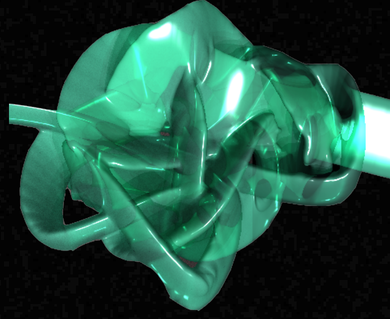

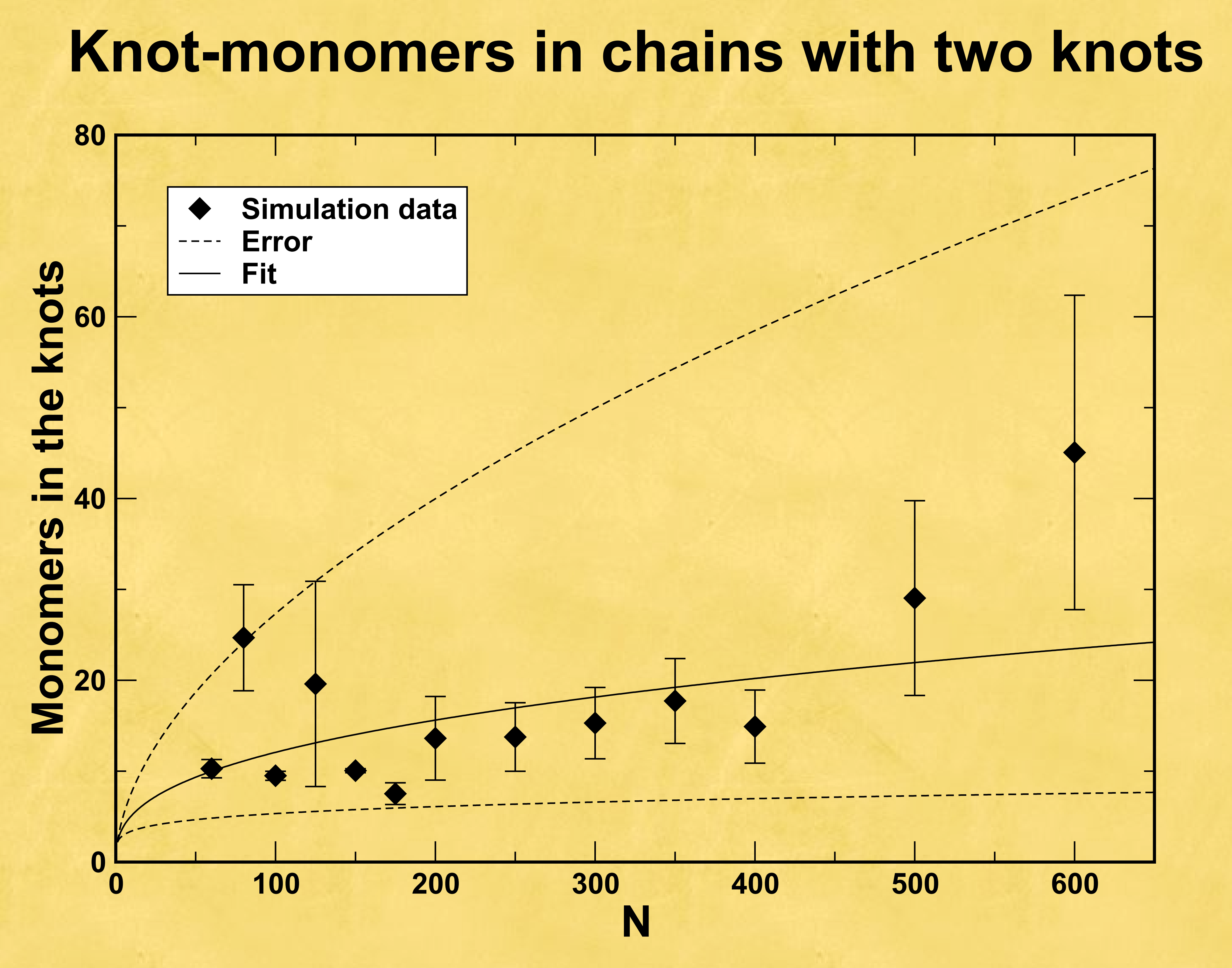

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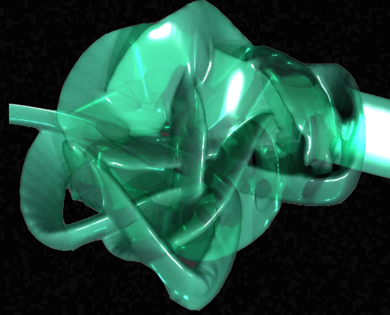
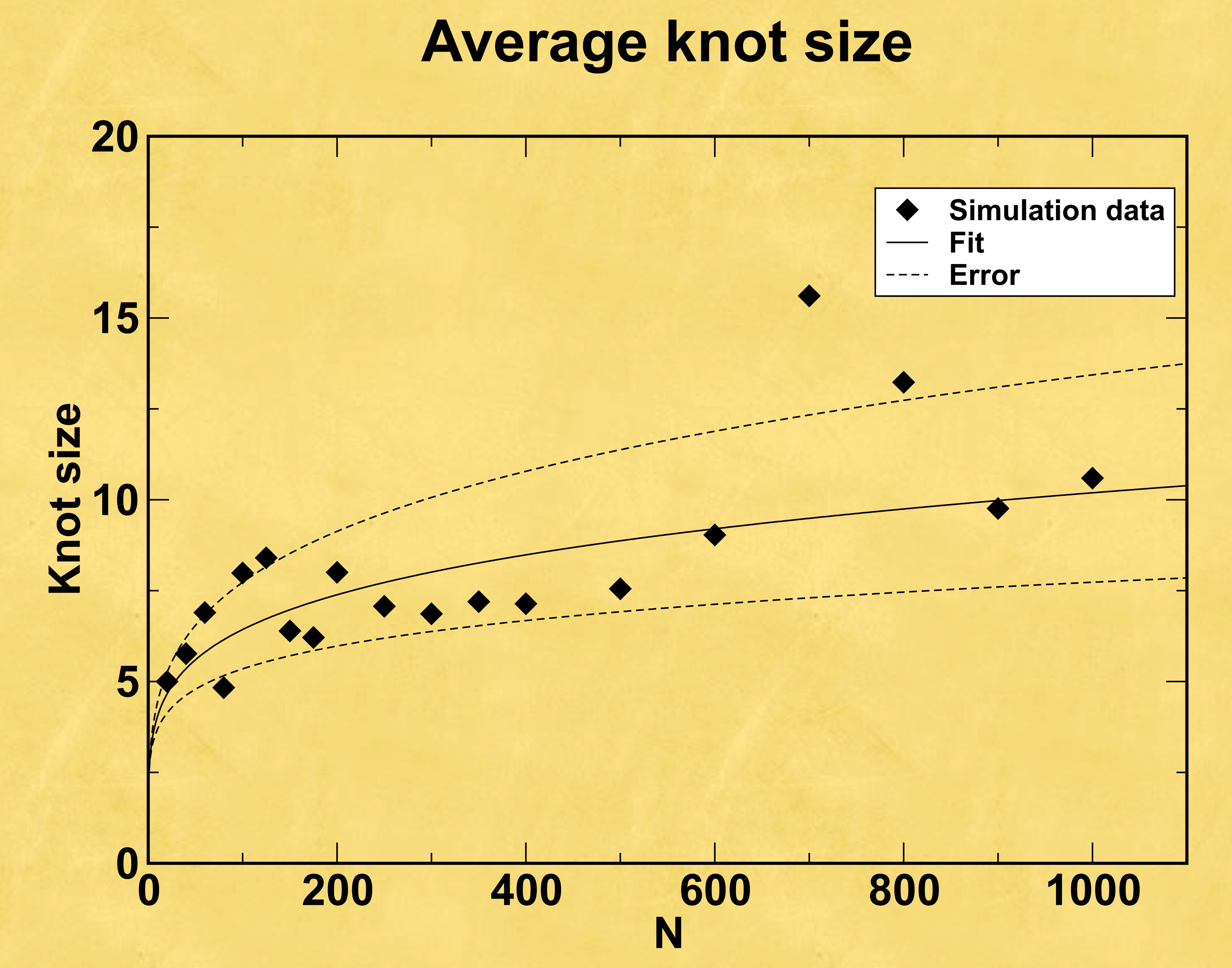
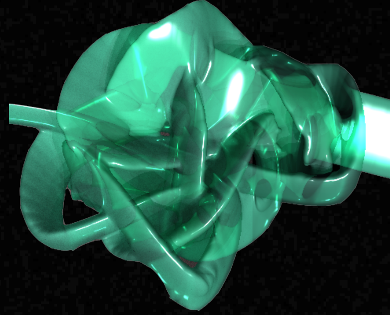




Summary



- Situtation still undecided concerning the average crossing number.
- Knot statistics also needs to be improved.

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Thank you for your attention!