Polymer task

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December 20, 2023

In the next table the theoretical results, extracted from this website, are presented. The scaling coefficients for Rp and Rg are the same because these magnitudes both measure the distance of an ending of the polymer with the initial position. In the case of Rp is the ending monomer, in the case of Rg is a virtual monomer in the center of mass of the system.

Ideal polymer		
	2D	**3D**
Rp^2/Rg^2	1	1

(a) Scaling for ideal polymer

Rosebluth polymer		
	2D	**3D**
Rp^2/Rg^2	1.5	1.2

(b) Scaling for Rosebluth polymer

Table 1: Scaling exponent for both types of polymers

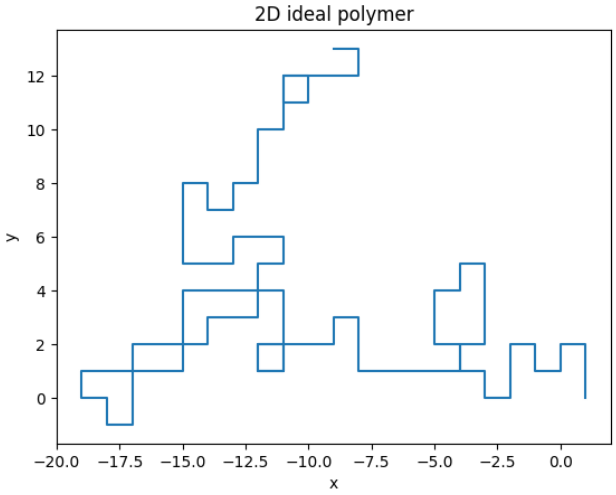
1 Ideal polymer

1.1 2D

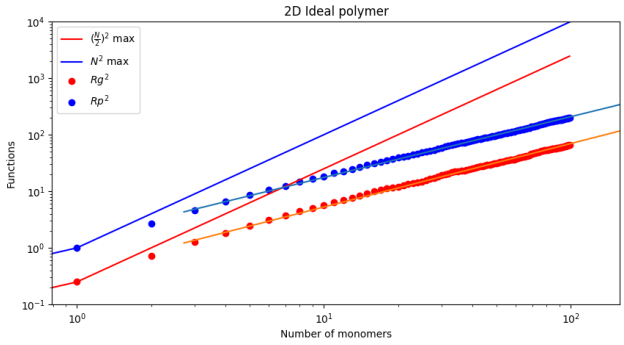
Lines in light blue and orange are the linear adjustment lines. Their respective slope is written in the next table with their correspodent relative error. The plot is in logarithmic scale because the dependence of both magnitudes with the number of monomers is exponential, so a logarithmic plot allows us to obtain the slope coeficient in an easier way.

2D ideal polymer			
Rp^2	1.07	**Error**	7.39%
Rg^2	1.12	**Error**	12.18%

Table 2: 2D ideal polymer: Computational values for Rp^2 and Rg^2.



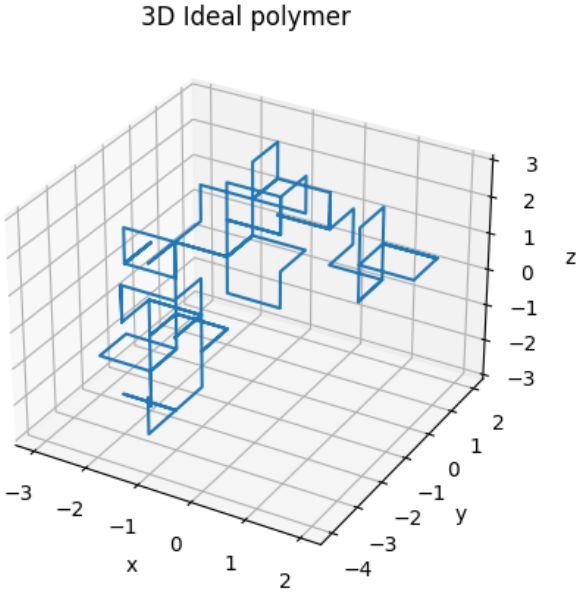
(a) 2D polymer



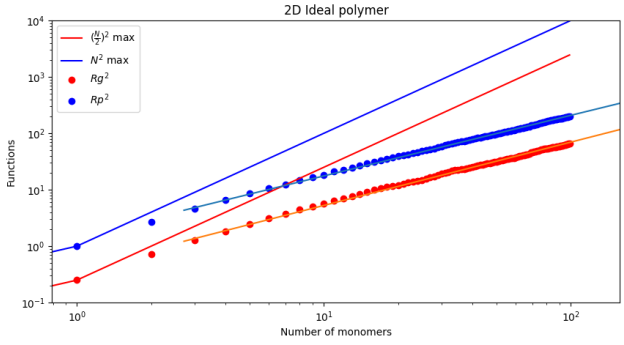
(b) Statistical computing of Rp^2 y Rg^2 adjusted to a line by lineal regression

Figure 1: 2D ideal polymer graphs

1.2 3D



(a) 3D ideal polymer



(b) Statistical computing of Rp^2 y Rg^2 adjusted to a line by lineal regression

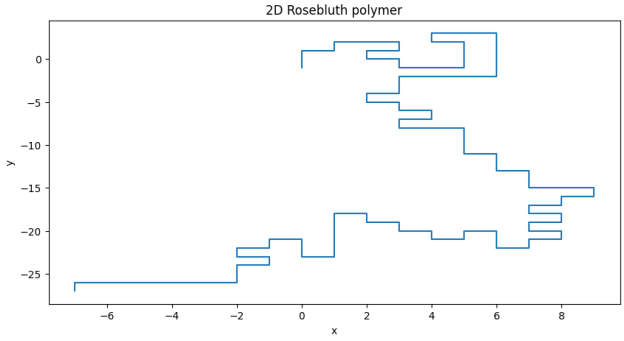
Figure 2: 3D ideal polymer graphs

3D ideal polymer			
Rp^2	0.96	**Error**	3.52%
Rg^2	0.99	**Error**	0.74%

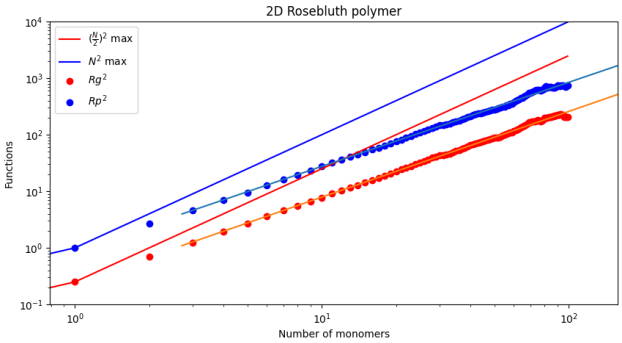
Table 3: 2D ideal polymer: Computational values for Rp^2 and Rg^2.

2 Rosebluth polymer

2.1 2D



(a) 2D Rosebluth polymer



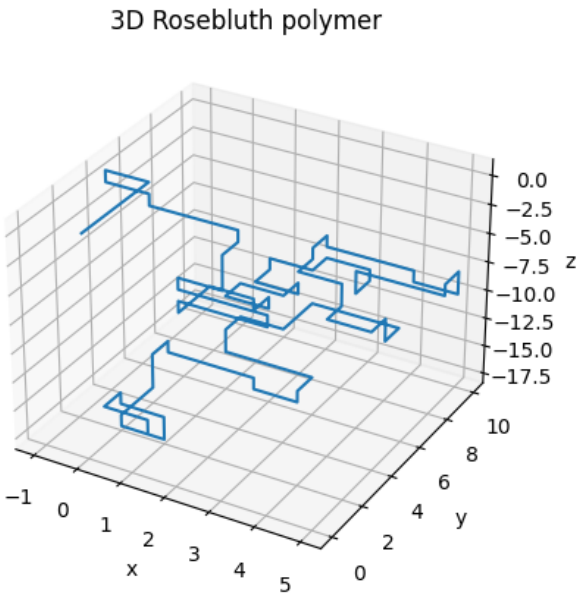
(b) 2D Rosebluth polymer: Comparison of theoretical and computational values for Rp^2 and Rg^2.

Figure 3: 2D Rosebluth polymer graphs

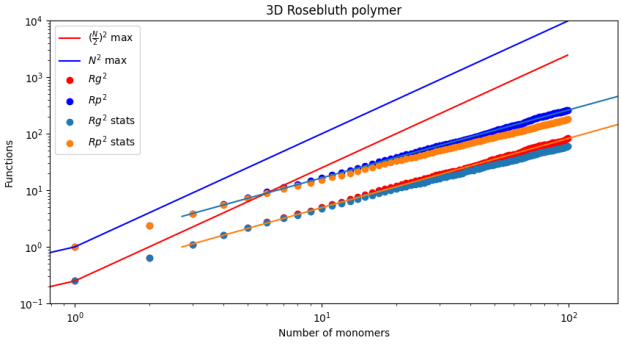
2D Rosebluth polymer			
Rp^2	1.43	**Error**	6.82%
Rg^2	1.46	**Error**	3.93%

Table 4: 2D Rosebluth polymer: Computational values for Rp^2 and Rg^2.

2.2 3D



(a) 3D Rosebluth polymer



(b) 3D Rosebluth polymer: Comparison of theoretical and computational values for Rp^2 and Rg^2. Scatter plots in orange and blue are Rp^2 and Rg^2 having done the ideal polymer statistical analysis.

Figure 4: 3D Rosebluth polymer graphs

3D Rosebluth polymer			
Rp^2	1.19	**Error**	1.34%
Rg^2	1.21	**Error**	1.433%

Table 5: 3D Rosebluth polymer: Computational values for Rp^2 and Rg^2.

Additionally, it has been performed the statistical analysis made for the ideal polymers,which does not take into account the weighting of each link.

3D Rosebluth polymer			
Rp^2	1.09	**Error**	11.03%
Rg^2	1.13	**Error**	7%

Table 6: 3D Rosebluth polymer: Computational values for Rp^2 and Rg^2 using ideal polymer statistical analysis

3 Conclusion

Th algorithms perform exactly the required type of polymer in each case, i.e. the ideal polymer can cross itself but not go back and the self-avoiding polymer can not cross itself.

However, computational results of Rp^2 and Rg^2 vary in accuracy between different models and different dimentions.
In the case of the ideal polymer, we find the computational errors produce are lesser in the 3D model. This could be due to the random nature of the creation of the polymer, as in different code executions we obtain different results and errors. The same pattern happens in the Rosebluth model; the 3D system is more accurate than the 2D one. However we can observe adding weights in computing Rp^2 and Rg^2 gives a better result than performing a standard averaging. By giving more weight to monomers which have more possible future configurations we benefit those positions which make the polymer grow, because those are the monomers who make Rp^2 and Rg^2 change appreciatively.