Simulación molecular

Índice

Algoritmos de simulación
- Deterministas vs estocásticos

Oscilador armónico
- Comprobación de los algoritmos

Potencial doble pozo

Polímero

Algoritmos de simulación

Dinámica Browniana

Ecuación diferencial estocástica

$$m\frac{d^2\vec{r}}{dt^2} = -\eta\frac{d\vec{r}}{dt} - \vec{\nabla}V(\vec{r}) + \xi(t)$$

Necesidad de desarrollar algoritmos estocásticos

Al igual que deterministas, velocidad vs precisión

Algoritmos de simulación

$$\boxed{v_{i+1} = v_i + hf(x_i, v_i, t_i)} + \boxed{(c_0 h)^{1/2}\xi}$$

Determinista

Estocástica

$h = \Delta t$

$c_0 = 2\eta K_B T$

Algoritmos de simulación

$$x_{i+1} = x_i + v_i bh + \frac{bh}{2m}\left[\mathrm{f}(\mathrm{x_i}, \mathrm{v_i}, \mathrm{t_i})h + \boxed{(c_0 h)^{1/2}\xi}\right]$$

$$v_{i+1} = av_i + \frac{h}{2m}\left(af(x_i, v_i, t_i) + f(x_{i+1}, v_i, t_i)\right) + \boxed{\frac{b}{m}(c_0 h)^{1/2}\xi}$$

$$a = \cancelto{1}{\frac{1 - \frac{\eta h}{2m}}{1 + \frac{\eta h}{2m}}} \quad ; \quad b = \cancelto{1}{\frac{1}{1 + \frac{\eta h}{2m}}}$$

Determinista

Estocástica

Algoritmos de simulación

$$
\begin{aligned}
g_{1x} &= v_i + \boxed{(c_0 h)^{1/2}\xi_2} \\
g_{1v} &= f\left(x_i, v_i + \boxed{(c_0 h)^{1/2}\xi_2}\right) \\
g_{2x} &= v_i + g_{1v}h \\
g_{2v} &= f\left(x_i + g_{1x}h + \boxed{(c_0 h)^{1/2}\xi_1}, v_i + g_{1v}h + \boxed{(c_0 h)^{1/2}\xi_2}\right)
\end{aligned}
$$

$$
\begin{aligned}
x_{i+1} &= x_i + h[A_1 g_{1x} + A_2 g_{2x}] \\
v_{i+1} &= v_i + h[A_1 g_{1v} + A_2 g_{2v}] + \boxed{(c_0 h)^{1/2}\xi_2}
\end{aligned}
$$

Pautas de programación

Programación modular

Cada algoritmo debe ser capaz de funcionar por su cuenta

Calcular constantes usadas más de una vez una única vez

Lanzar un algoritmo debe ser una llamada a una función encargada de todo

Multi-Threading

- Varias simulaciones a la vez (una por núcleo) ✓
- "Dividir" el polímero en sub-partes y simular cada una por separado ✗

Oscilador armónico

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x$$

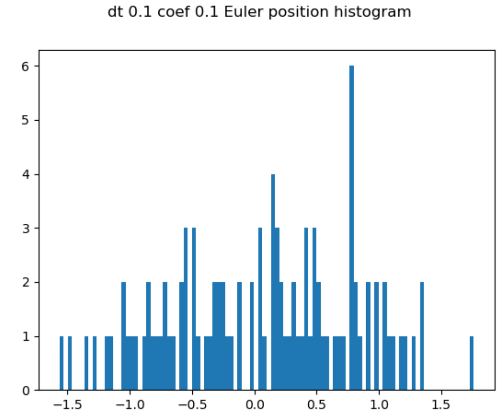
Oscilador armónico

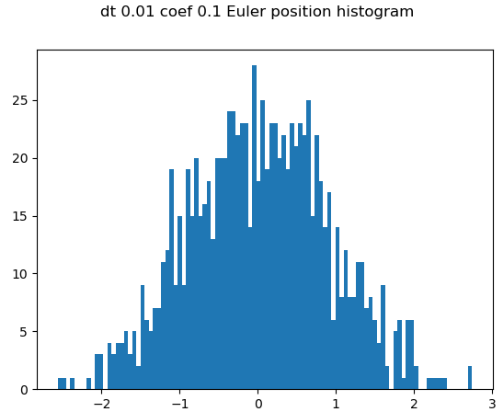
Comprobar el funcionamiento de los distintos algoritmos

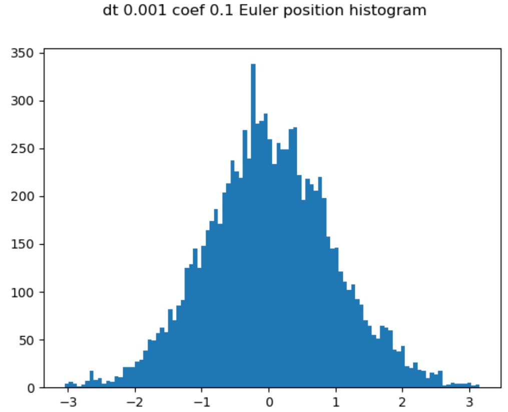
Diferencias en los resultados

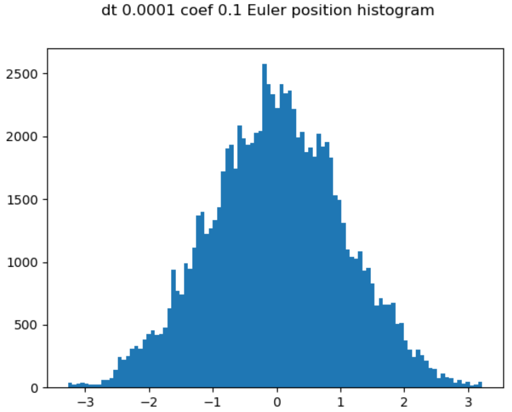
- Según el algoritmo
- Según valor del paso del tiempo
- Según valor del damping

Oscilador armónico

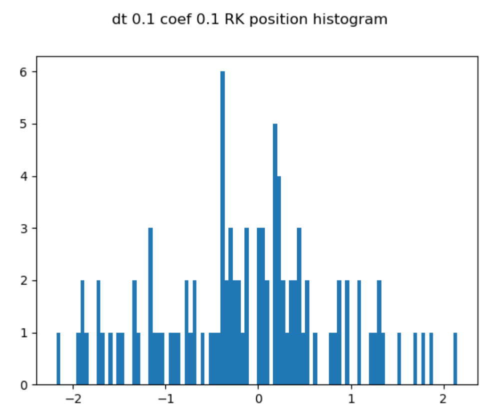


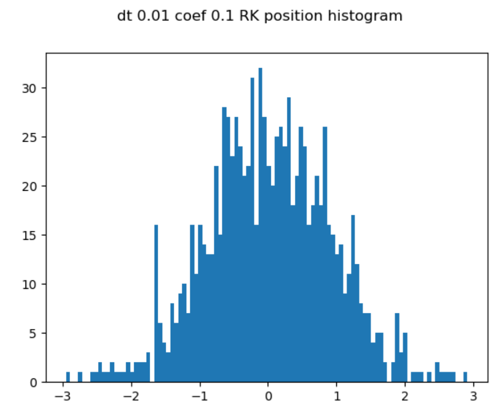


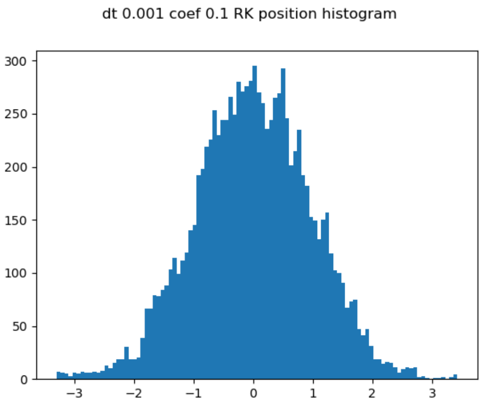


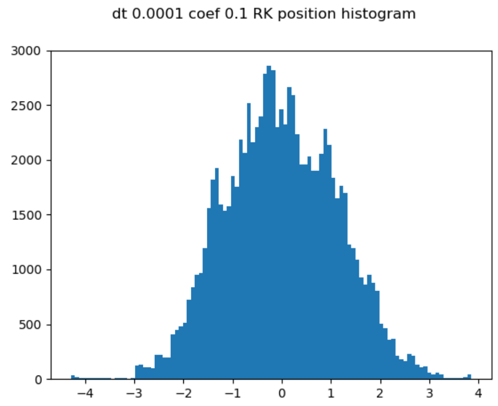


Oscilador armónico

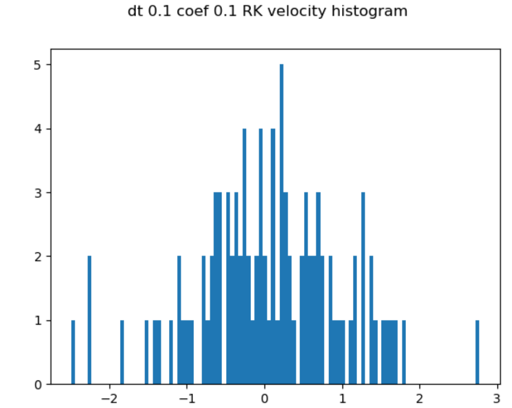


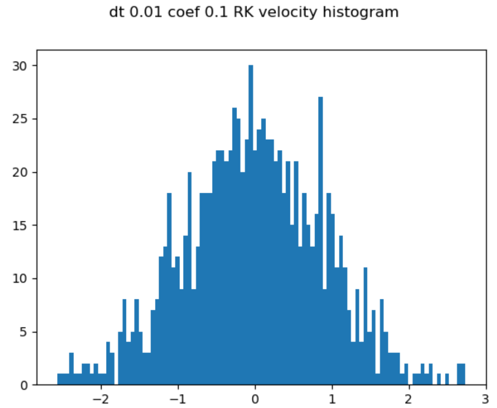


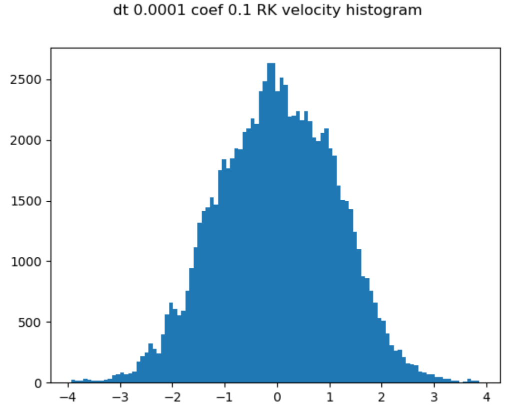


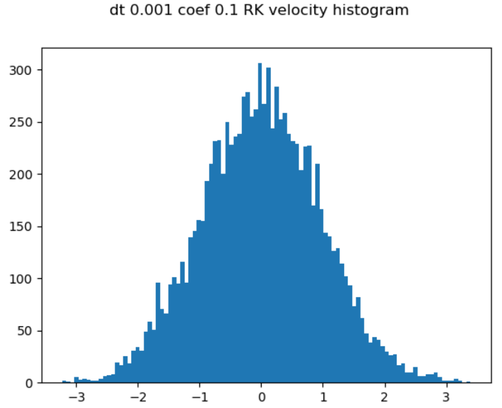


Oscilador armónico





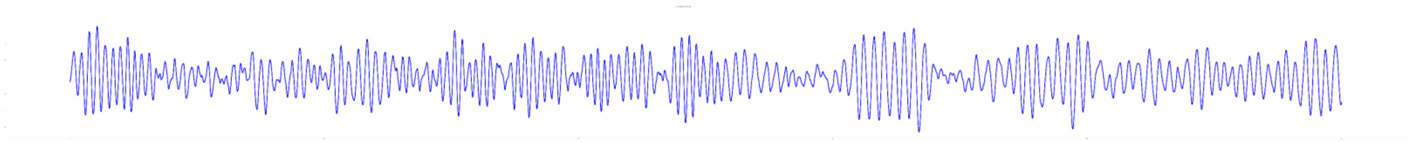




Oscilador armónico

Comparación de algoritmos

Euler

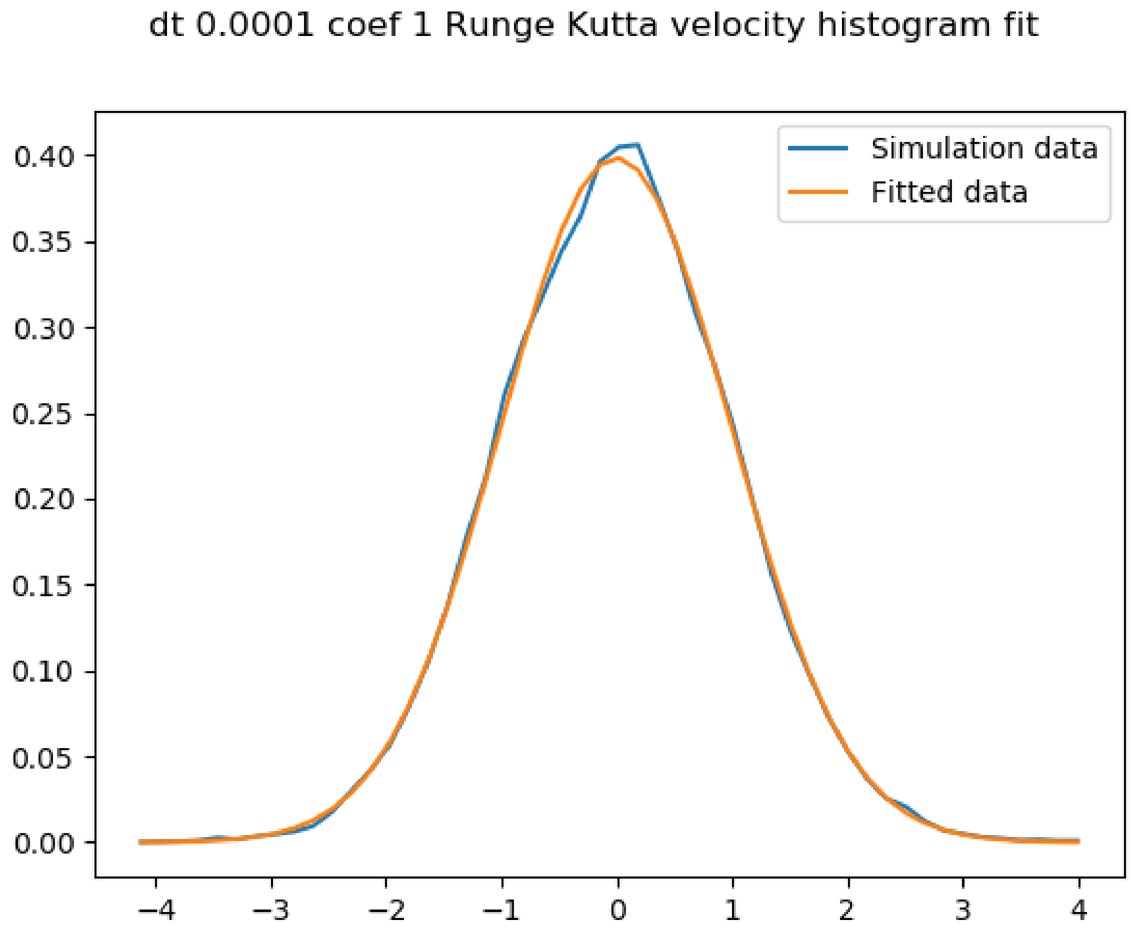


Verlet

RK

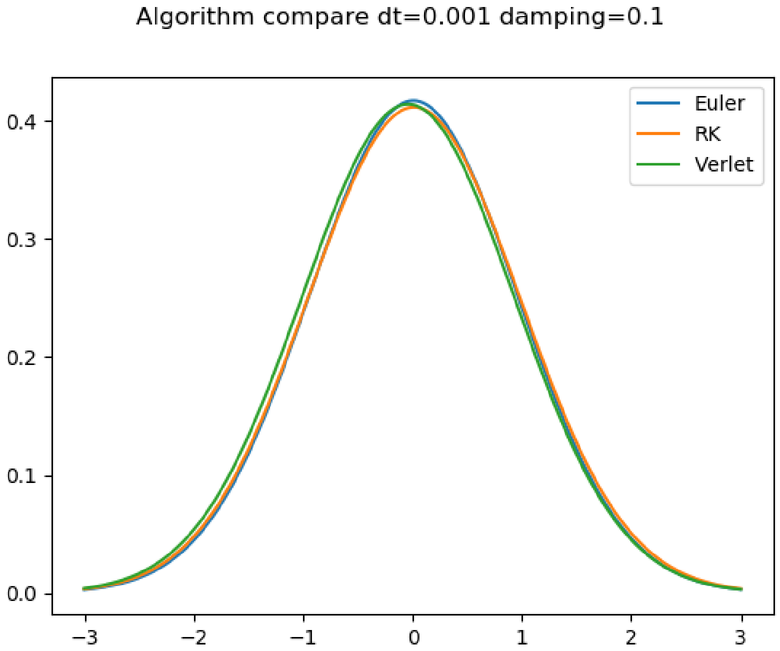
Oscilador armónico

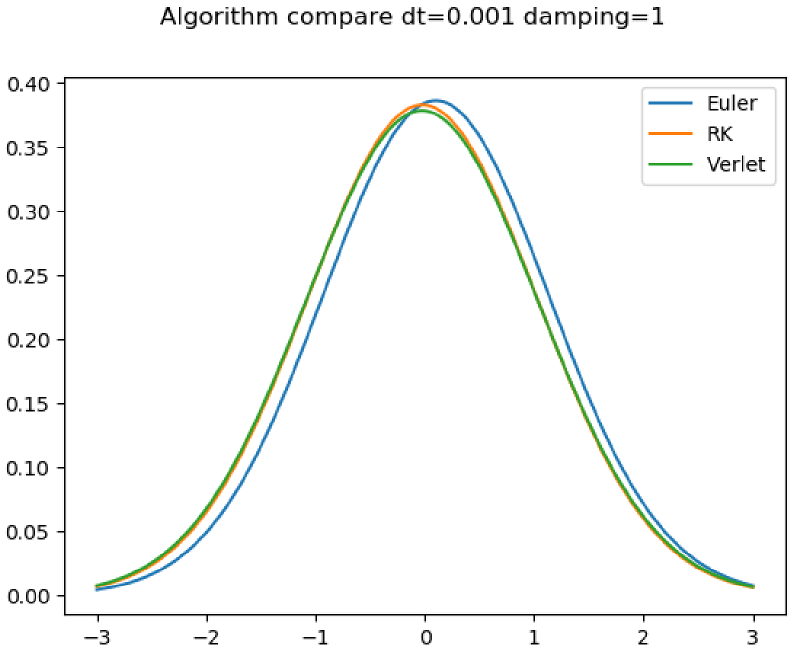
Comparación de algoritmos

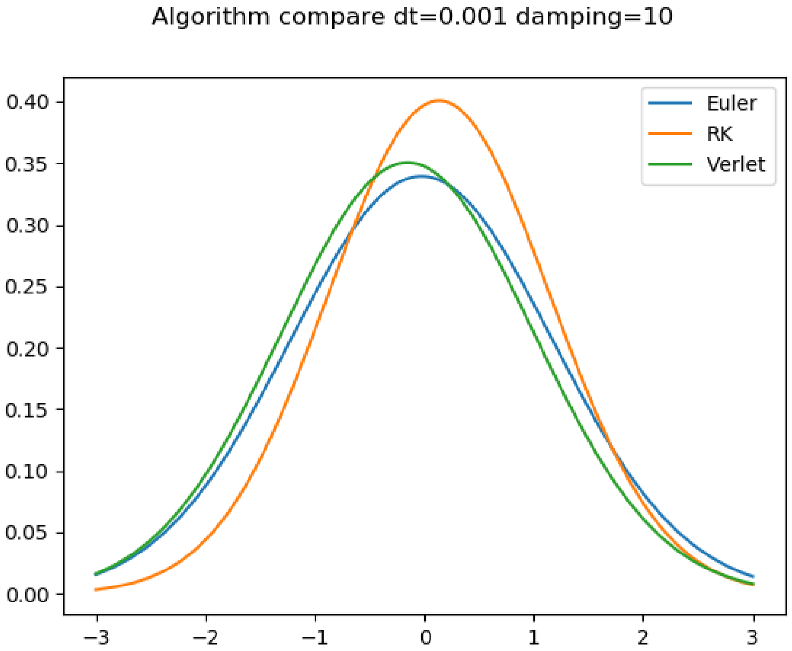


Oscilador armónico

Comparación de algoritmos

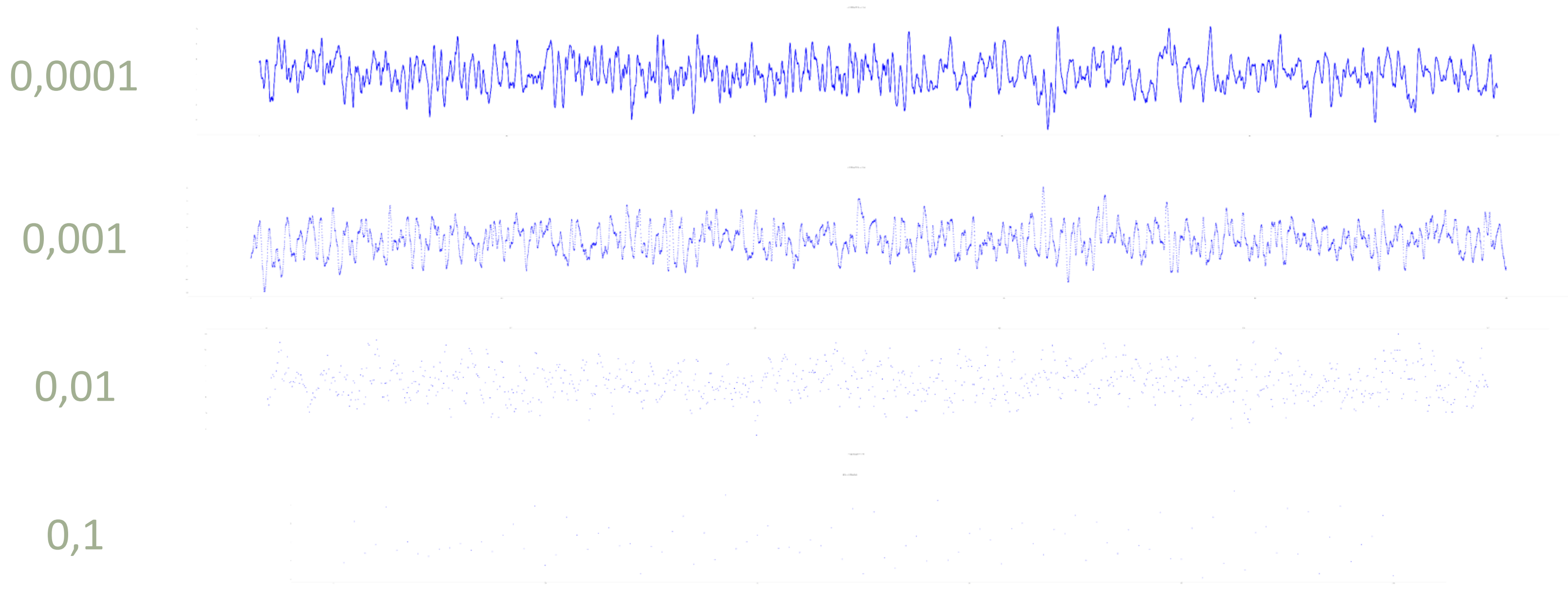






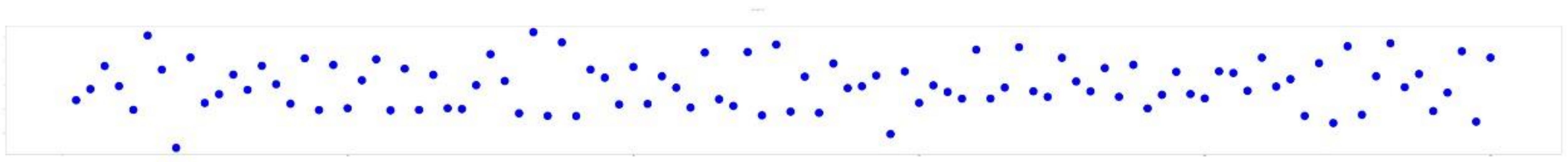
Oscilador armónico

Comparación de paso temporal



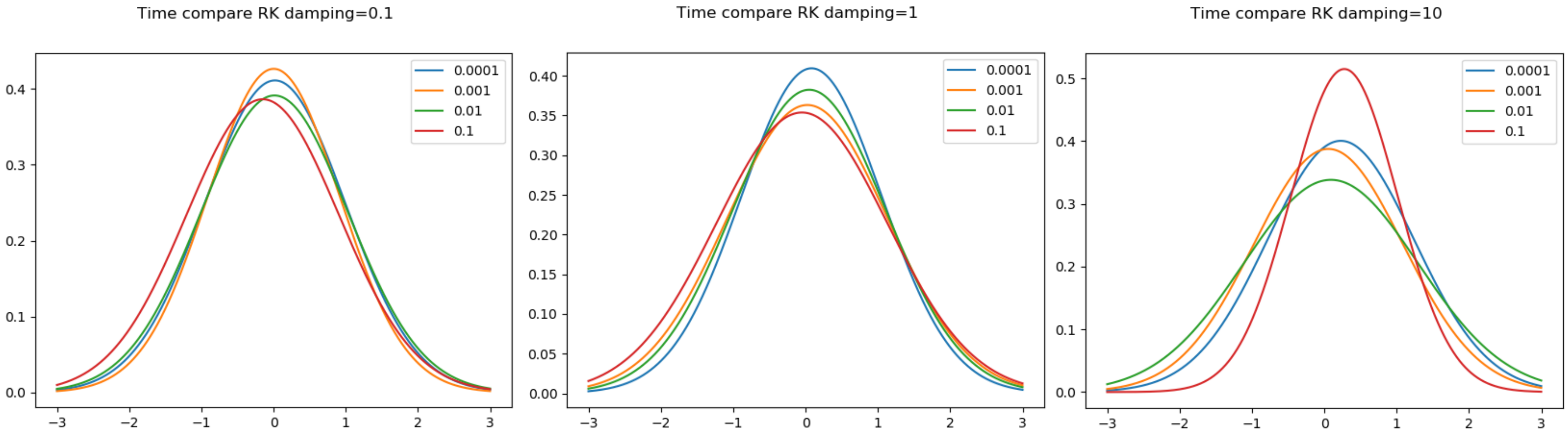
Oscilador armónico

Comparación de paso temporal



Oscilador armónico

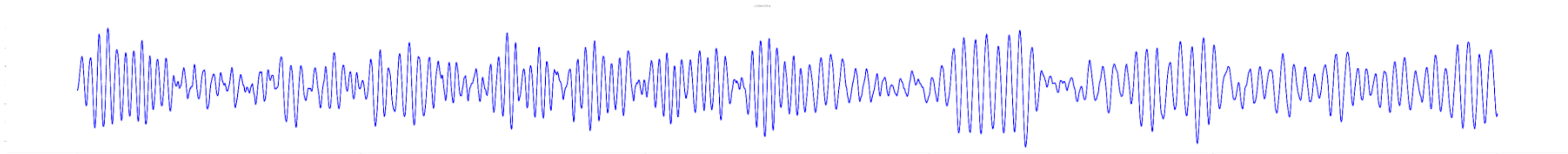
Comparación de paso temporal



Oscilador armónico

Comparación de término de damping

0,1



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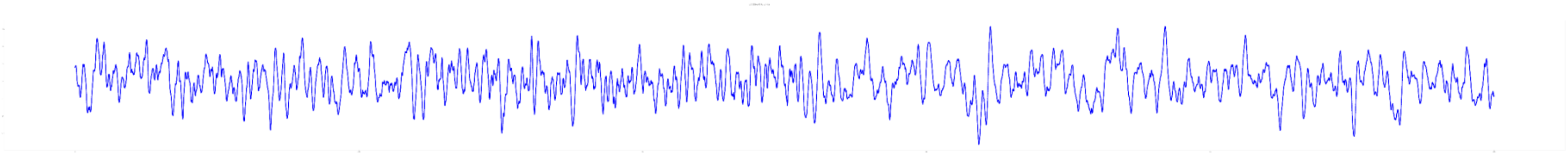

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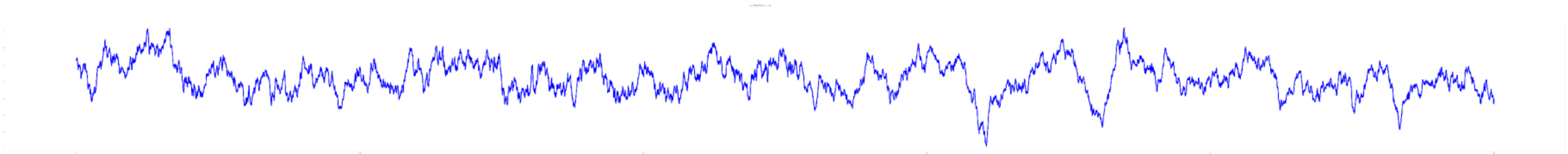
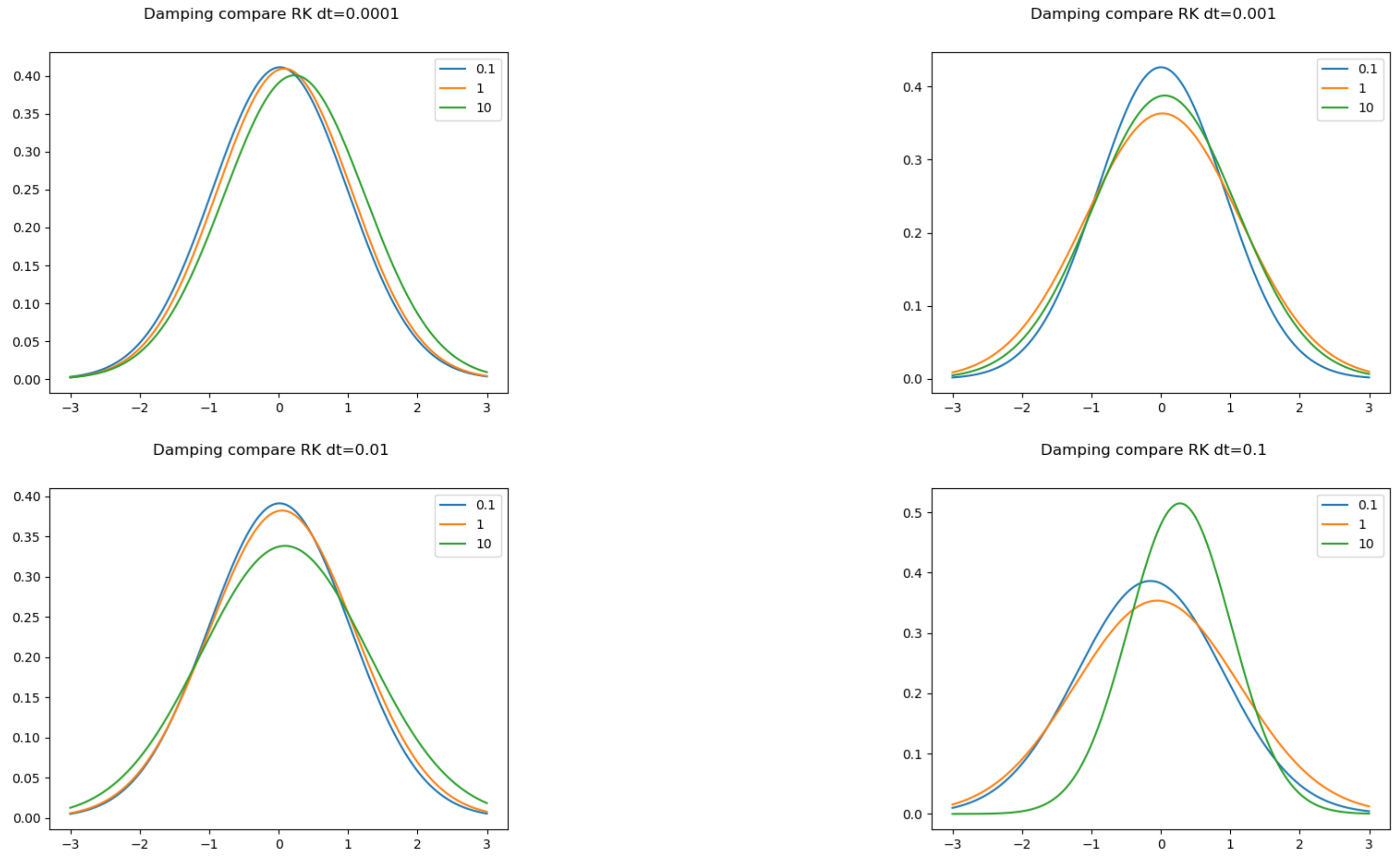


Oscilador armónico

Comparación de término de damping



Euler	$h = 10^{-4}$	$h = 10^{-3}$	$h = 10^{-2}$	$h = 10^{-1}$
$\gamma = 0,1$	$E_c = 0{,}55 \pm 0{,}37$ $E_p = 0{,}56 \pm 0{,}39$	$E_c = 0{,}46 \pm 0{,}31$ $E_p = 0{,}47 \pm 0{,}41$	$E_c = 0{,}51 \pm 0{,}68$ $E_p = 0{,}52 \pm 0{,}70$	$E_c = 0{,}43 \pm 0{,}37$ $E_p = 0{,}55 \pm 0{,}61$
$\gamma = 1$	$E_c = 0{,}50 \pm 0{,}42$ $E_p = 0{,}49 \pm 0{,}43$	$E_c = 0{,}52 \pm 0{,}57$ $E_p = 0{,}54 \pm 0{,}62$	$E_c = 0{,}51 \pm 0{,}67$ $E_p = 0{,}51 \pm 0{,}57$	$E_c = 0{,}54 \pm 0{,}75$ $E_p = 0{,}41 \pm 0{,}19$
$\gamma = 10$	$E_c = 0{,}49 \pm 0{,}49$ $E_p = 0{,}54 \pm 0{,}71$	$E_c = 0{,}52 \pm 0{,}52$ $E_p = 0{,}64 \pm 0{,}68$	$E_c = 0{,}56 \pm 0{,}68$ $E_p = 0{,}57 \pm 0{,}32$	$E_c = 0{,}97 \pm 2{,}89$ $E_p = 0{,}63 \pm 1{,}12$

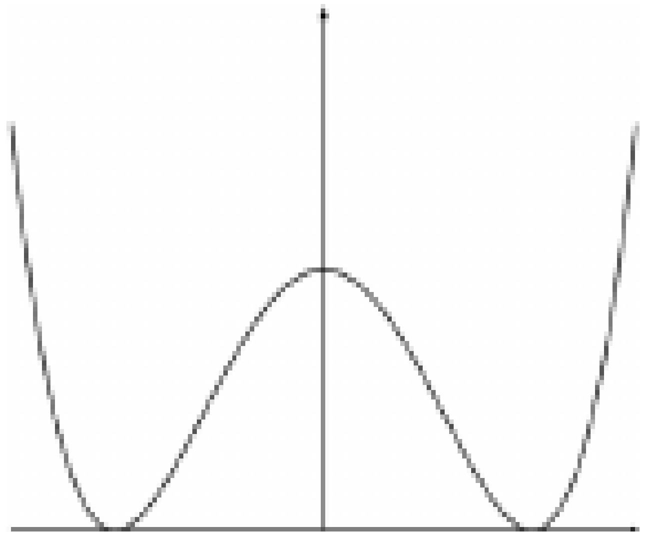
Verlet	$h = 10^{-4}$	$h = 10^{-3}$	$h = 10^{-2}$	$h = 10^{-1}$
$\gamma = 0,1$	$E_c = 0{,}46 \pm 0{,}42$ $E_p = 0{,}46 \pm 0{,}34$	$E_c = 0{,}44 \pm 0{,}29$ $E_p = 0{,}44 \pm 0{,}33$	$E_c = 0{,}49 \pm 0{,}42$ $E_p = 0{,}49 \pm 0{,}36$	$E_c = 0{,}56 \pm 0{,}52$ $E_p = 0{,}42 \pm 0{,}49$
$\gamma = 1$	$E_c = 0{,}47 \pm 0{,}42$ $E_p = 0{,}47 \pm 0{,}39$	$E_c = 0{,}52 \pm 0{,}53$ $E_p = 0{,}54 \pm 0{,}55$	$E_c = 0{,}52 \pm 0{,}54$ $E_p = 0{,}49 \pm 0{,}46$	$E_c = 0{,}40 \pm 0{,}31$ $E_p = 0{,}43 \pm 0{,}50$
$\gamma = 10$	$E_c = 0{,}49 \pm 0{,}50$ $E_p = 0{,}43 \pm 0{,}41$	$E_c = 0{,}50 \pm 0{,}51$ $E_p = 0{,}61 \pm 0{,}58$	$E_c = 0{,}51 \pm 0{,}52$ $E_p = 0{,}55 \pm 0{,}43$	$E_c = 0{,}43 \pm 0{,}21$ $E_p = 0{,}44 \pm 0{,}32$

RK	$h = 10^{-4}$	$h = 10^{-3}$	$h = 10^{-2}$	$h = 10^{-1}$
$\gamma = 0,1$	$E_c = 0{,}42 \pm 0{,}32$ $E_p = 0{,}51 \pm 0{,}34$	$E_c = 0{,}47 \pm 0{,}38$ $E_p = 0{,}47 \pm 0{,}42$	$E_c = 0{,}41 \pm 0{,}32$ $E_p = 0{,}41 \pm 0{,}31$	$E_c = 0{,}43 \pm 0{,}37$ $E_p = 0{,}45 \pm 0{,}36$
$\gamma = 1$	$E_c = 0{,}51 \pm 0{,}52$ $E_p = 0{,}50 \pm 0{,}49$	$E_c = 0{,}52 \pm 0{,}49$ $E_p = 0{,}52 \pm 0{,}46$	$E_c = 0{,}46 \pm 0{,}42$ $E_p = 0{,}44 \pm 0{,}34$	$E_c = 0{,}54 \pm 0{,}41$ $E_p = 0{,}50 \pm 0{,}38$
$\gamma = 10$	$E_c = 0{,}50 \pm 0{,}48$ $E_p = 0{,}59 \pm 0{,}74$	$E_c = 0{,}50 \pm 0{,}47$ $E_p = 0{,}47 \pm 0{,}39$	$E_c = 0{,}42 \pm 0{,}31$ $E_p = 0{,}36 \pm 0{,}21$	$E_c = 0{,}36 \pm 0{,}23$ $E_p = 0{,}23 \pm 0{,}37$

Doble Pozo

Potencial usado:

$$V(x) = \tfrac{1}{2} B \, (x^2 - 1)^2$$



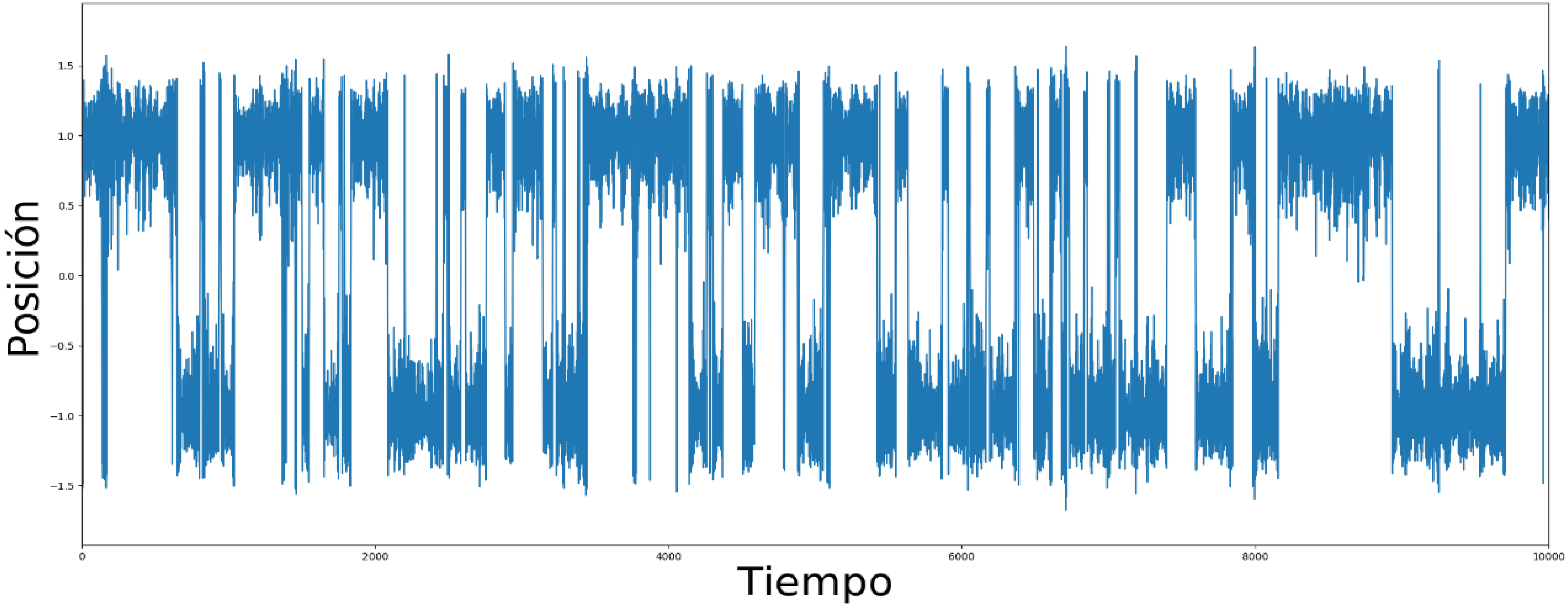
Comprobación de la equiparticion de la energía cinética

T	B	Eta	E_{cin}	E_{pot}
0.200	2.000	1.000	0.100	1.874
2.000	1.000	1.000	0.992	1.039
2.000	1.000	10.000	1.003	1.045
2.000	5.000	1.000	0.990	4.138

Tiempo de integración: 2E5
Paso temporal: 1E-2

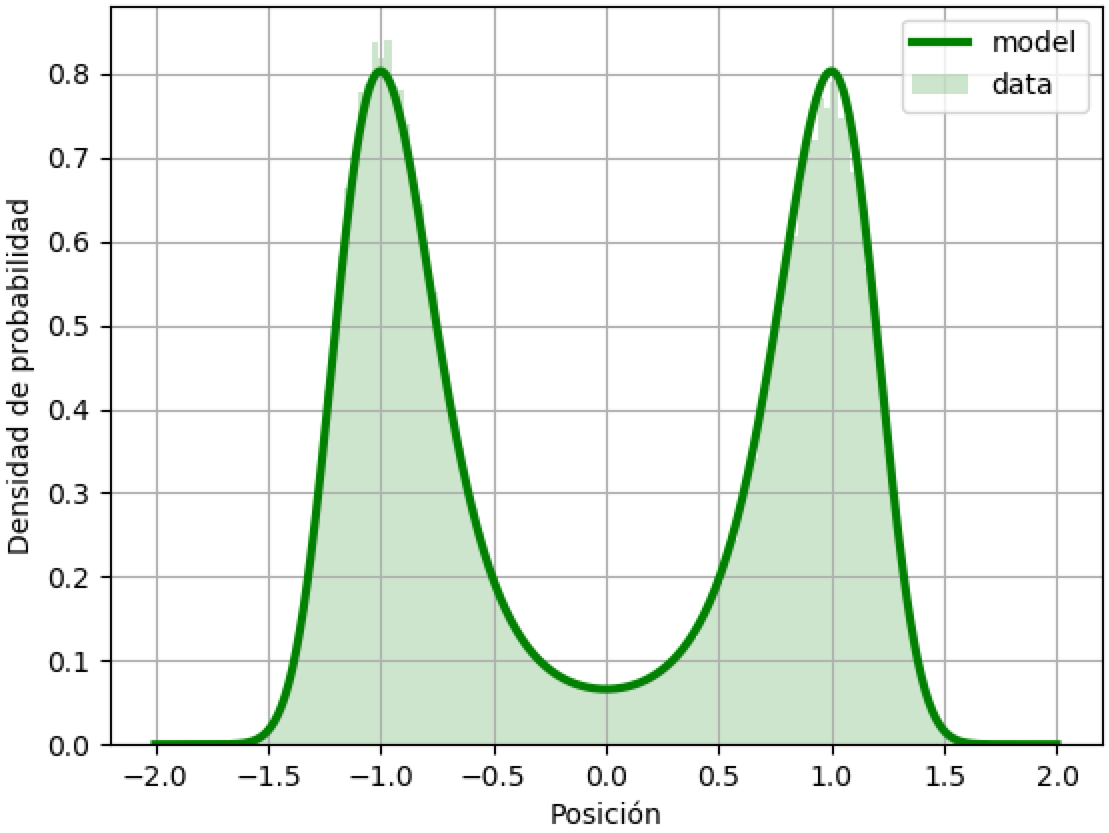
¿Qué ocurre si a altura de barrera fija variamos el "damping"?

T=0.2 B=1 Eta=0.1



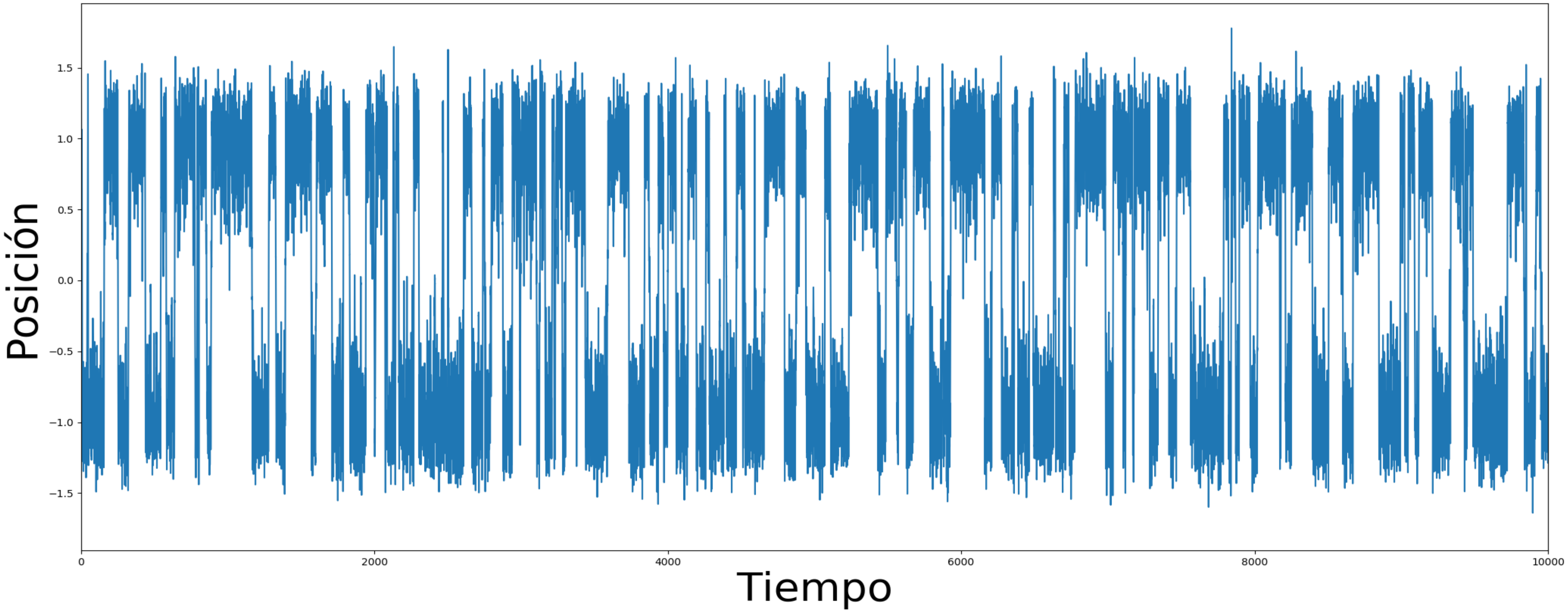
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
Posición
0
2000
4000
6000
8000
10000
Tiempo

T=0.2 B=1 Eta=0.1



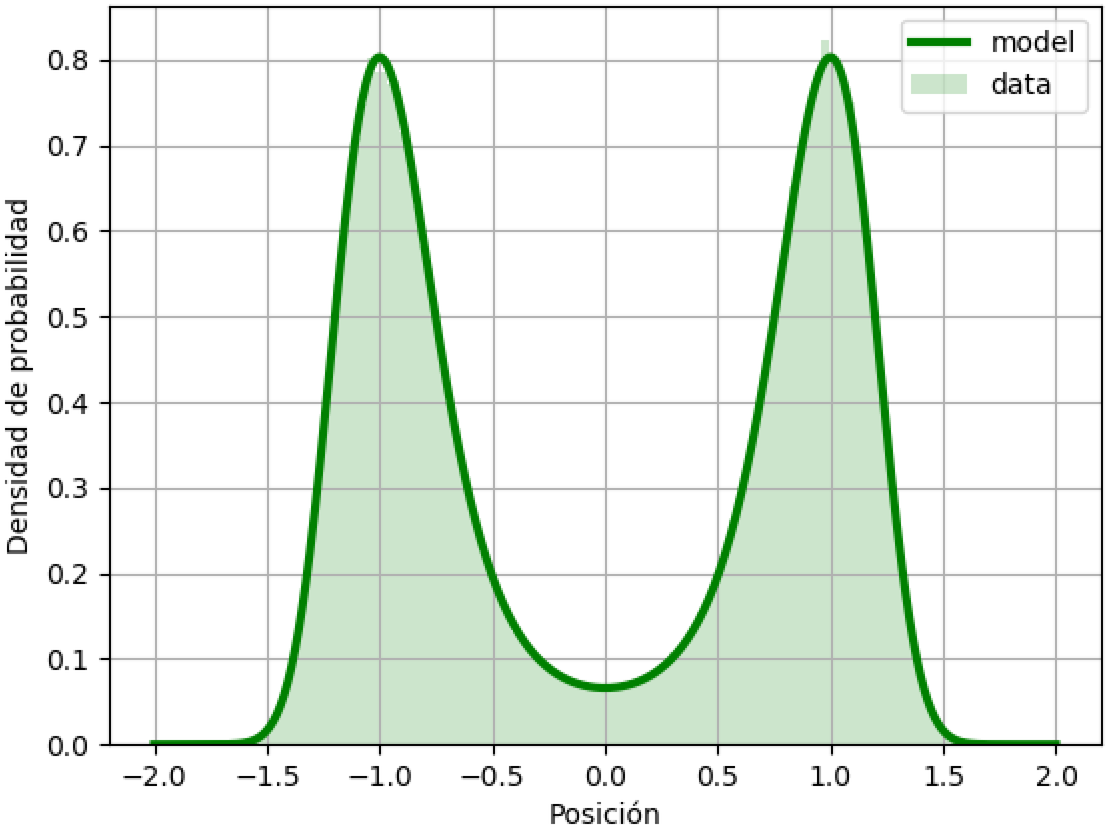
model
data
Densidad de probabilidad
Posición
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

T=0.2 B=1 Eta=1



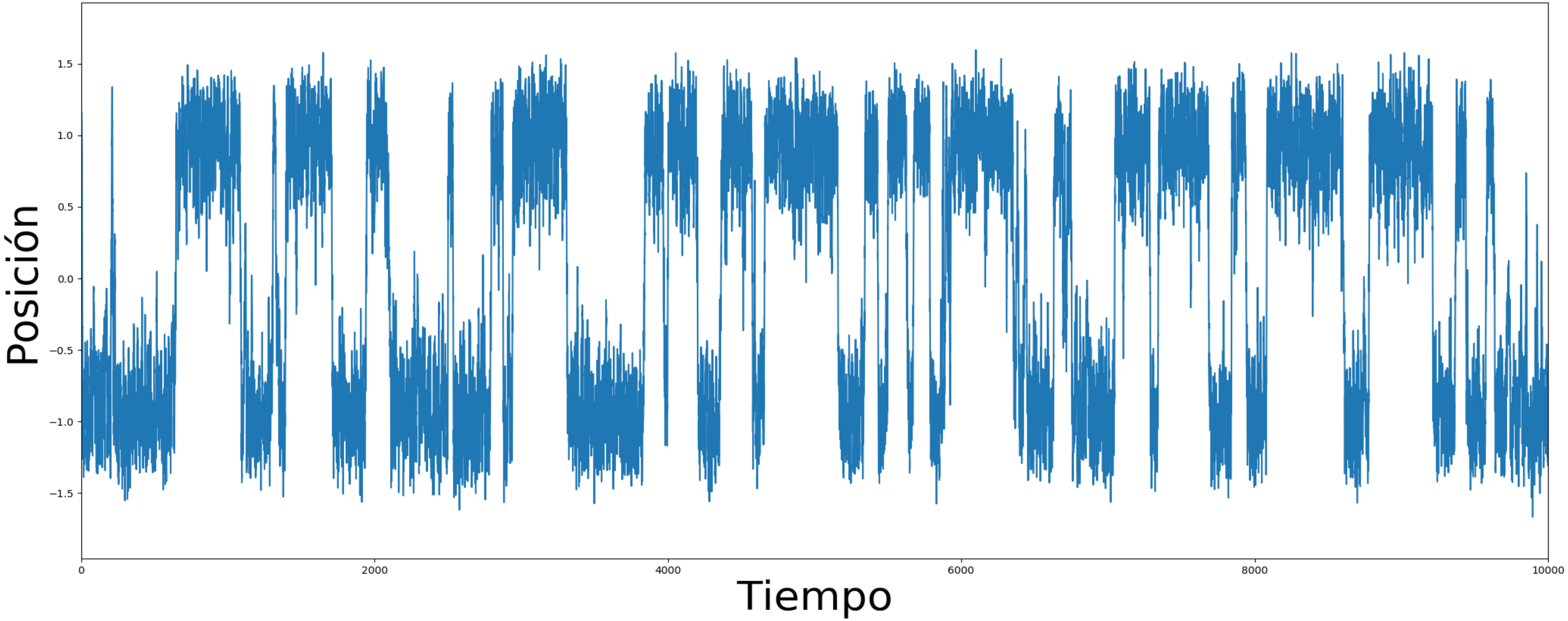
Posición
Tiempo
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
2000
4000
6000
8000
10000

T=0.2 B=1 Eta=1



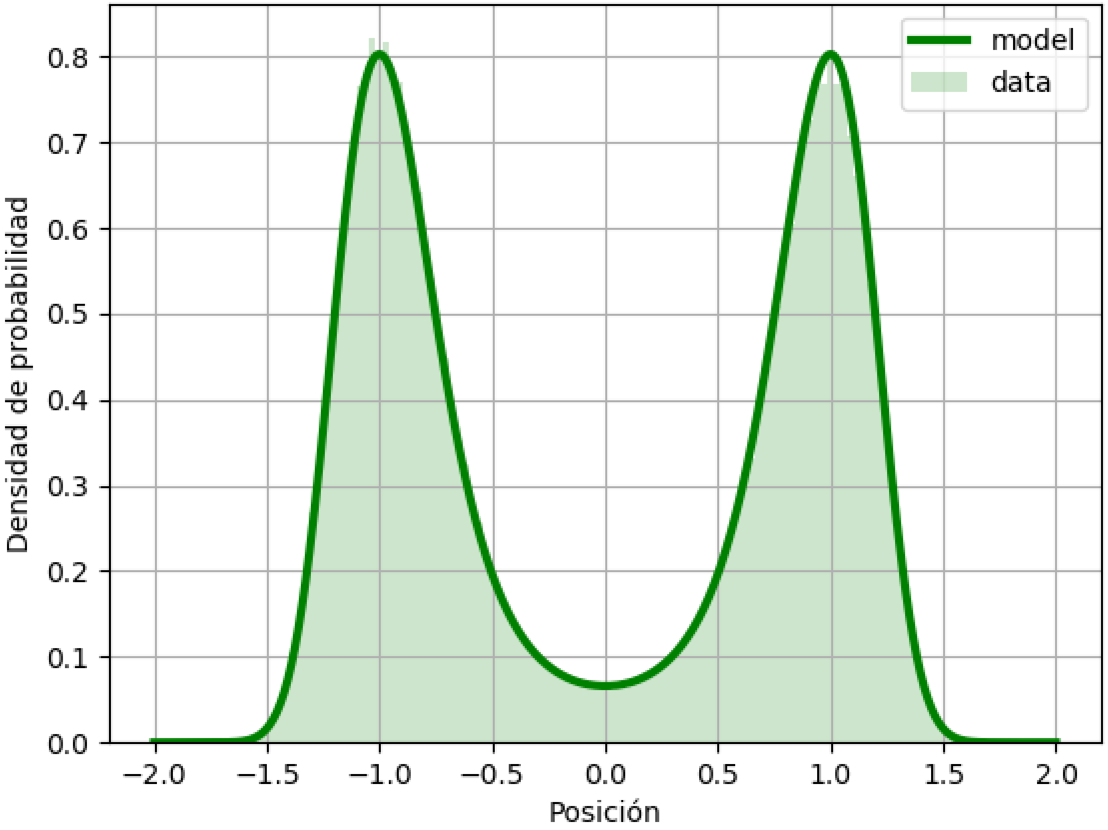
model
data
Densidad de probabilidad
Posición
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

T=0.2 B=1 Eta=5



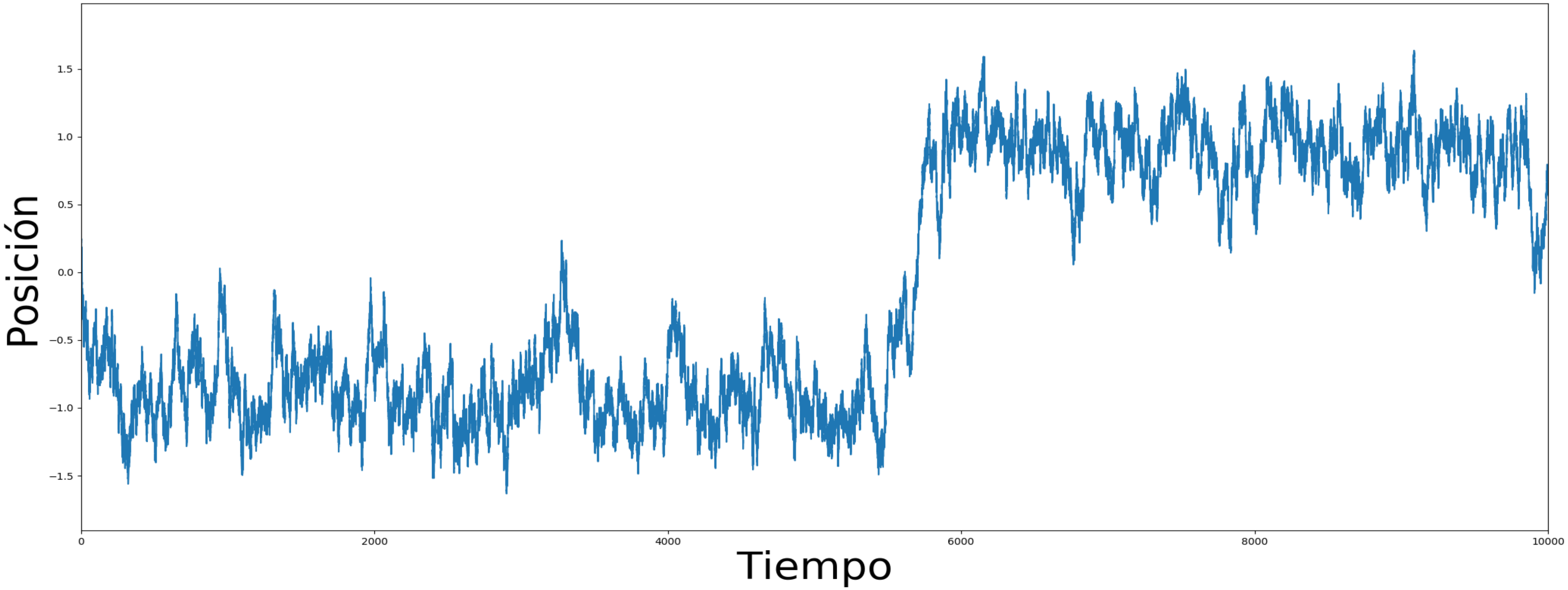
Posición
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
2000
4000
6000
8000
10000
Tiempo

T=0.2 B=1 Eta=5



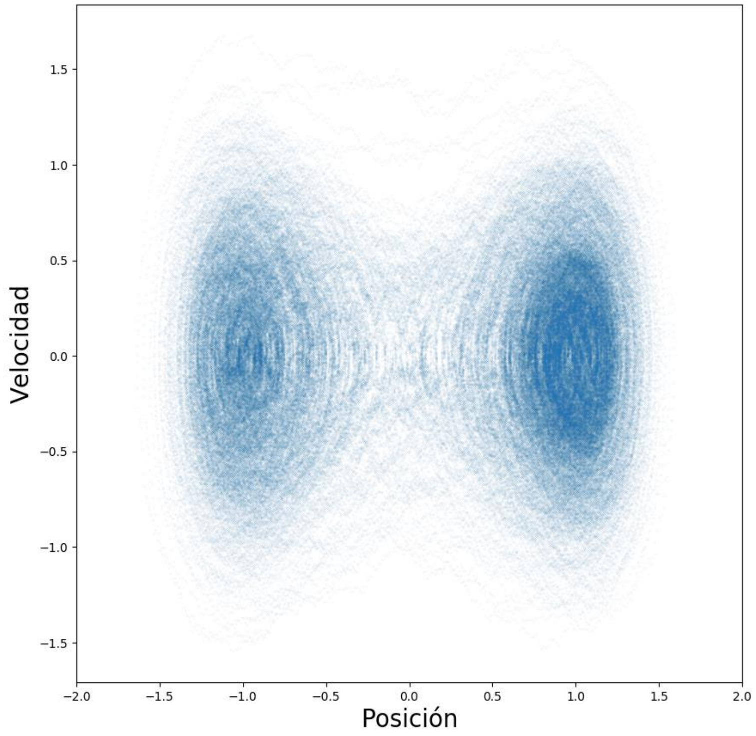
model
data
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Densidad de probabilidad
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
Posición

T=0.2 B=1 Eta=100

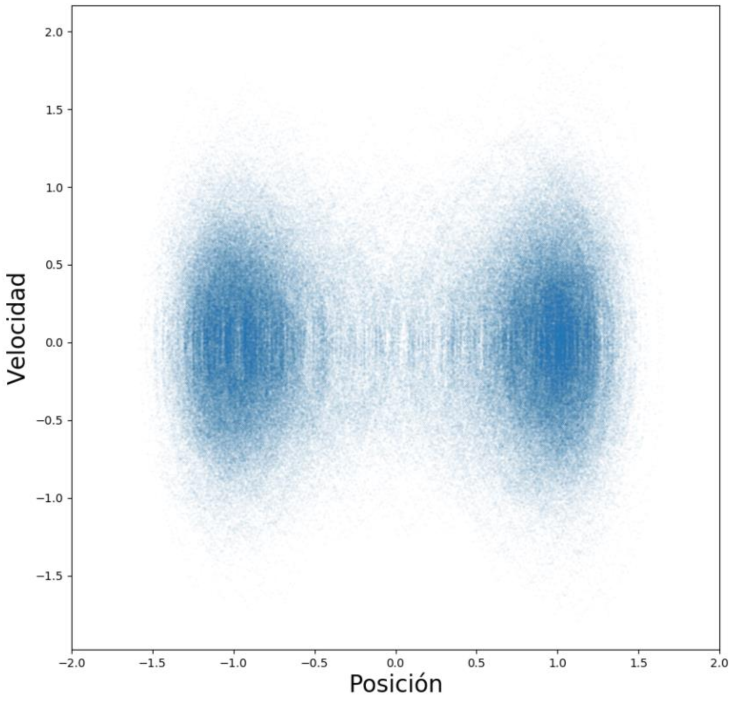


DIAGRAMAS DE FASE

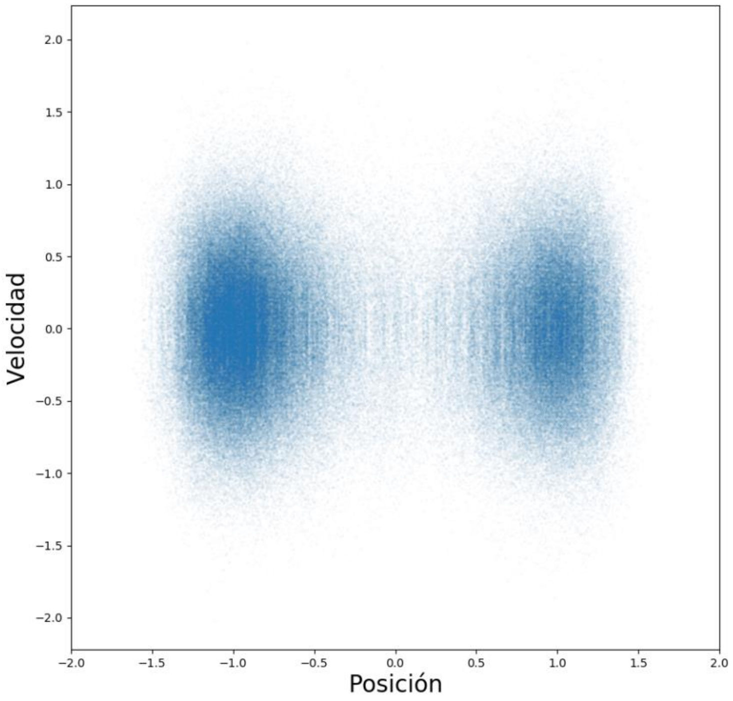
T=0.2 B=1
Eta=0.1



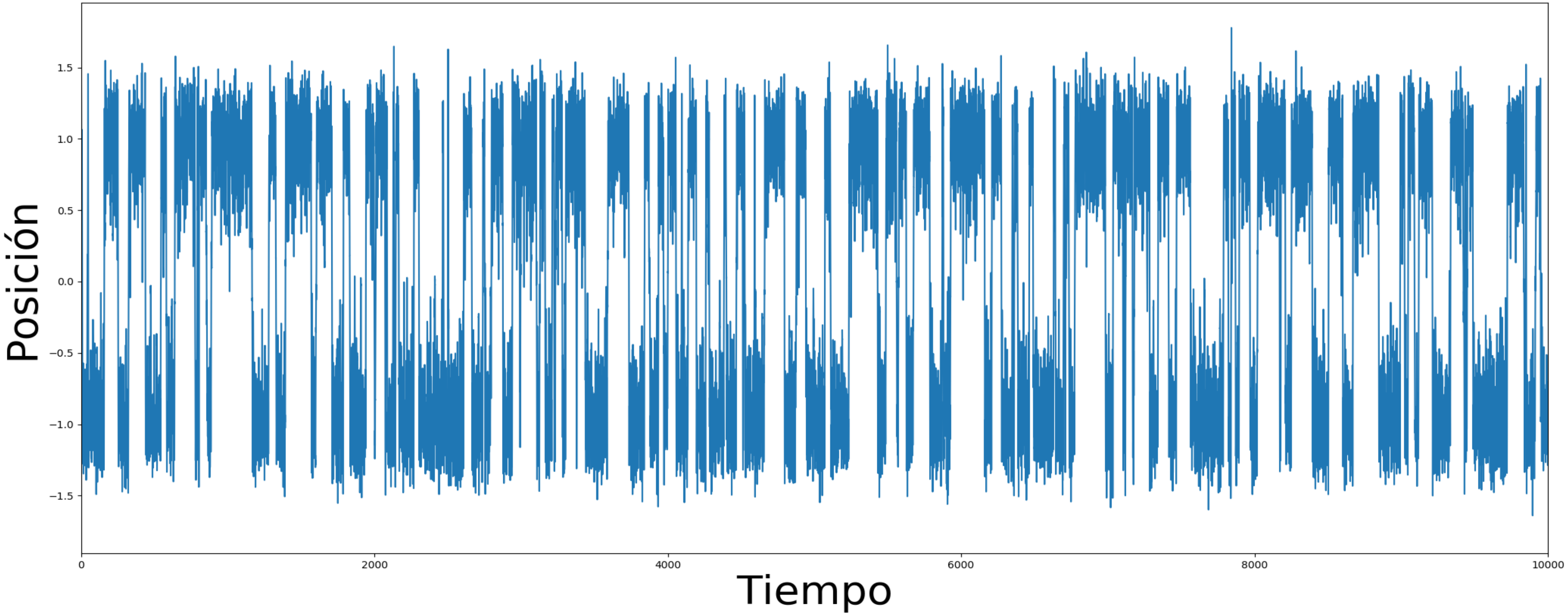
T=0.2 B=1
Eta=1



T=0.2 B=1
Eta=5

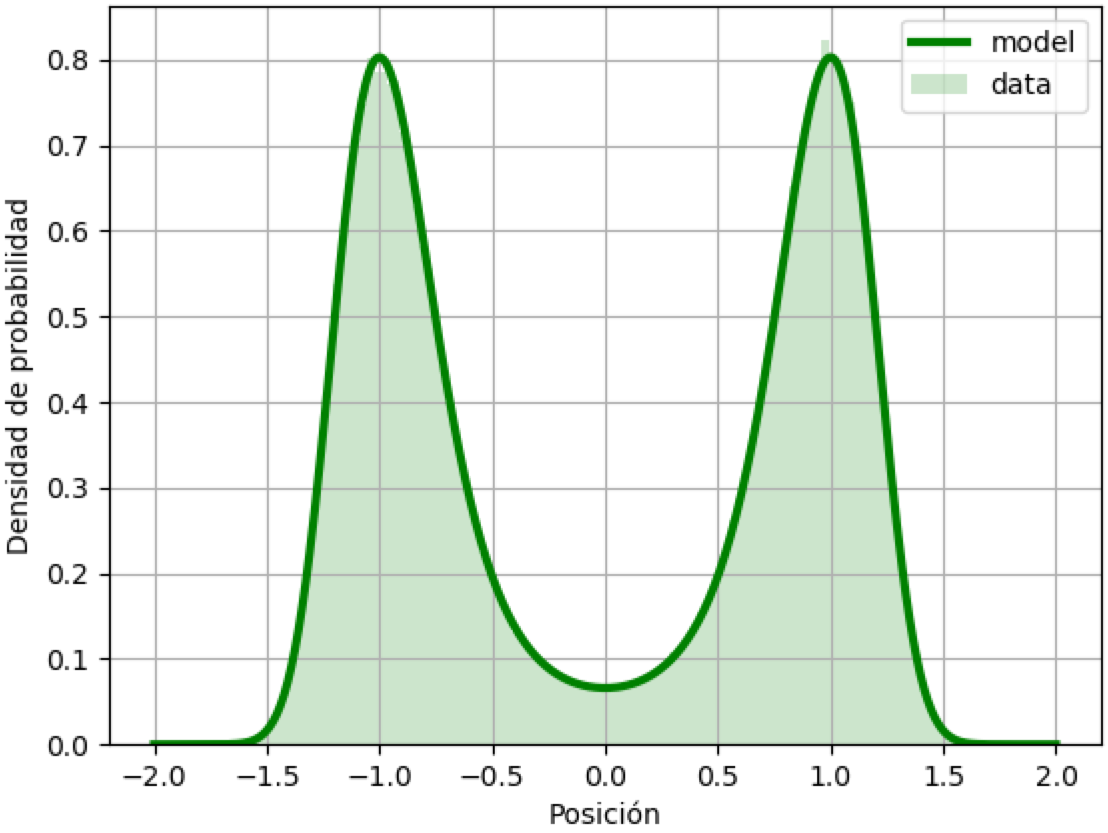


T=0.2 B=1 Eta=1



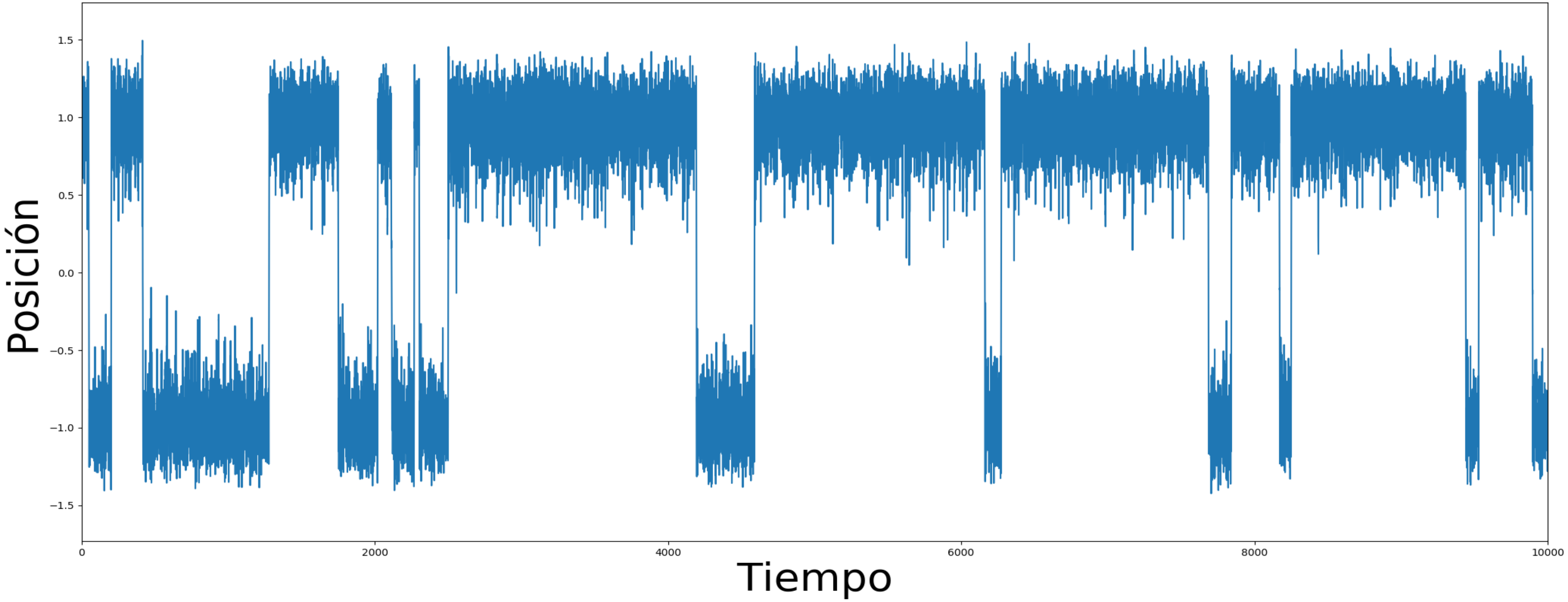
Posición
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
2000
4000
6000
8000
10000
Tiempo

T=0.2 B=1 Eta=1



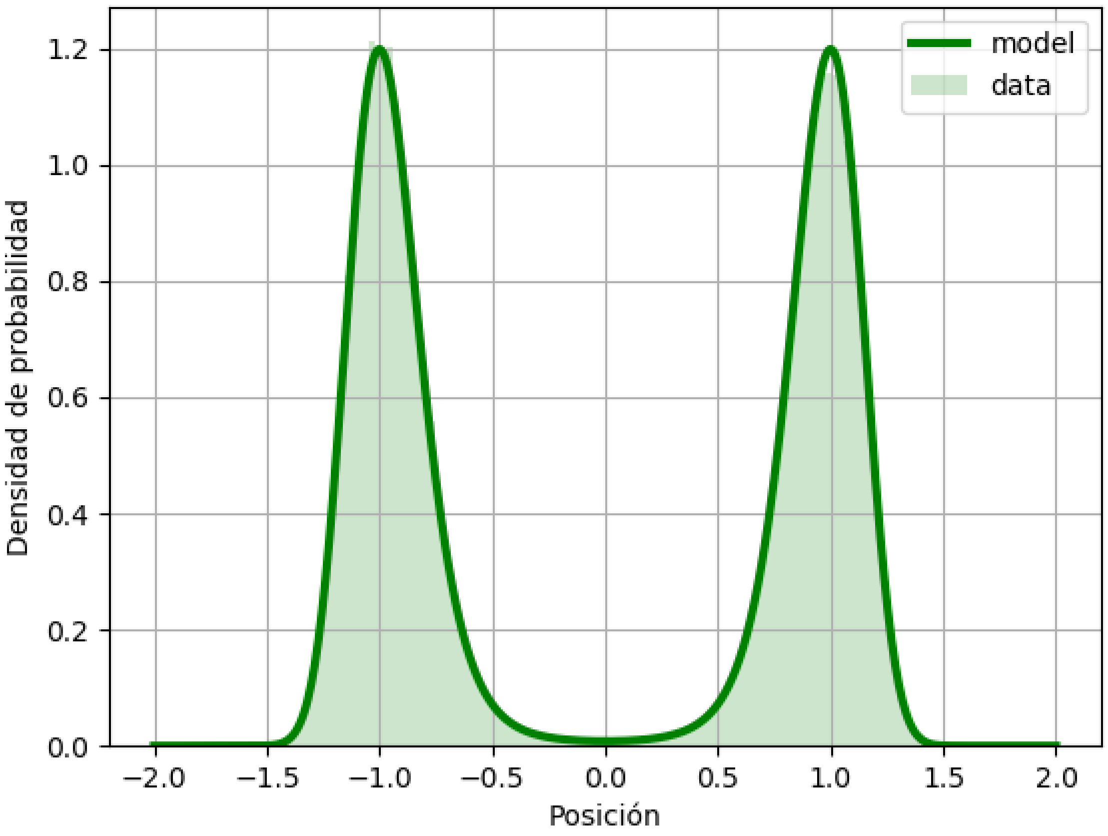
model
data
Densidad de probabilidad
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
Posición

T=0.2 B=2 Eta=1



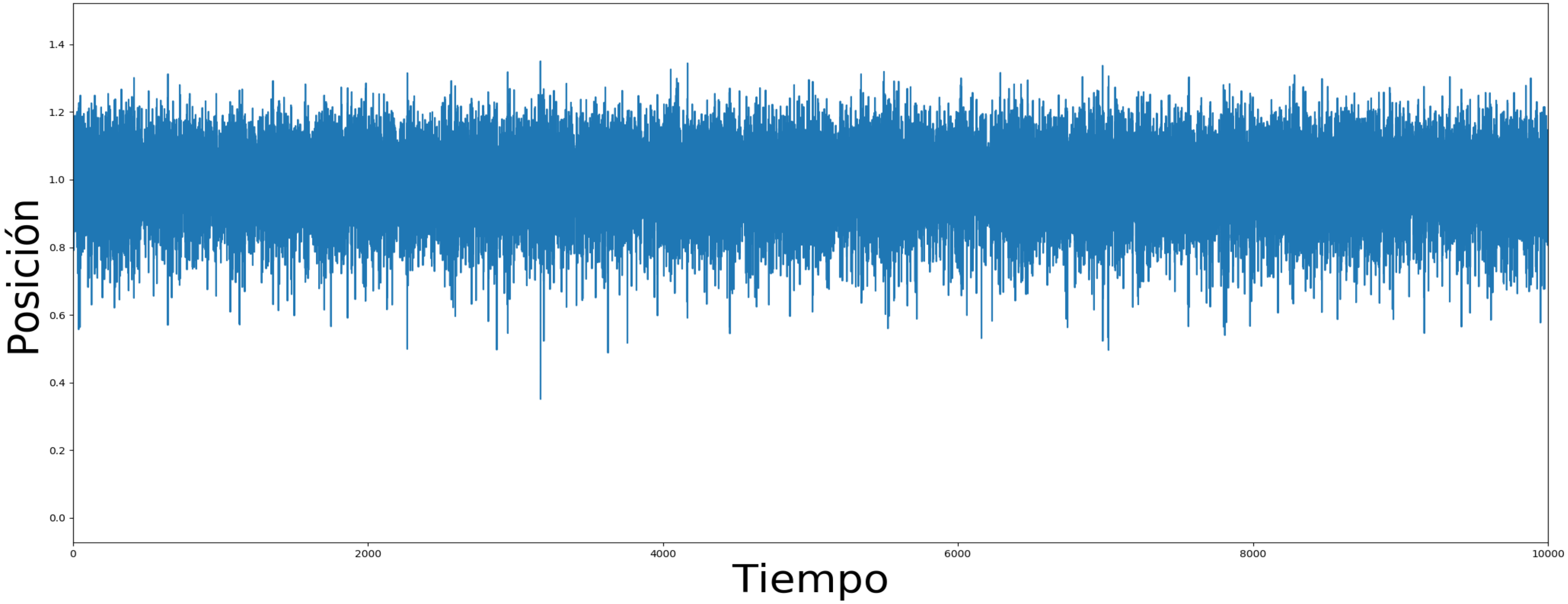
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
Posición
0
2000
4000
6000
8000
10000
Tiempo

T=0.2 B=2 Eta=1



model
data
Densidad de probabilidad
Posición
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

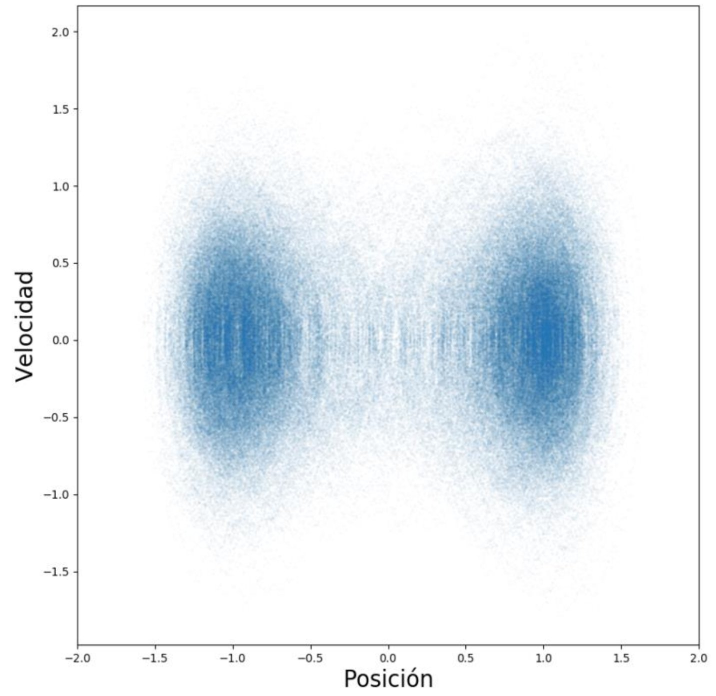
T=0.2 B=5 Eta=1



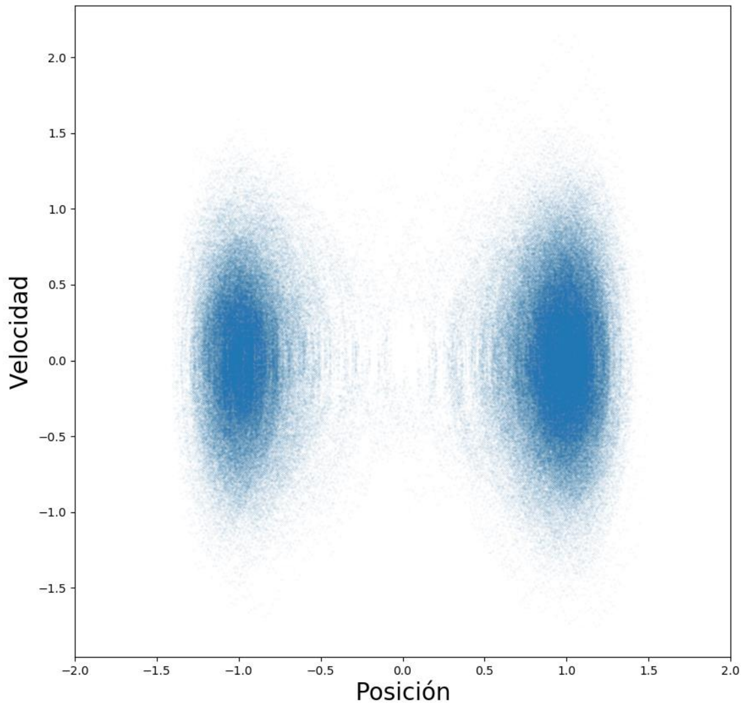
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Posición
0
2000
4000
6000
8000
10000
Tiempo

DIAGRAMAS DE FASE

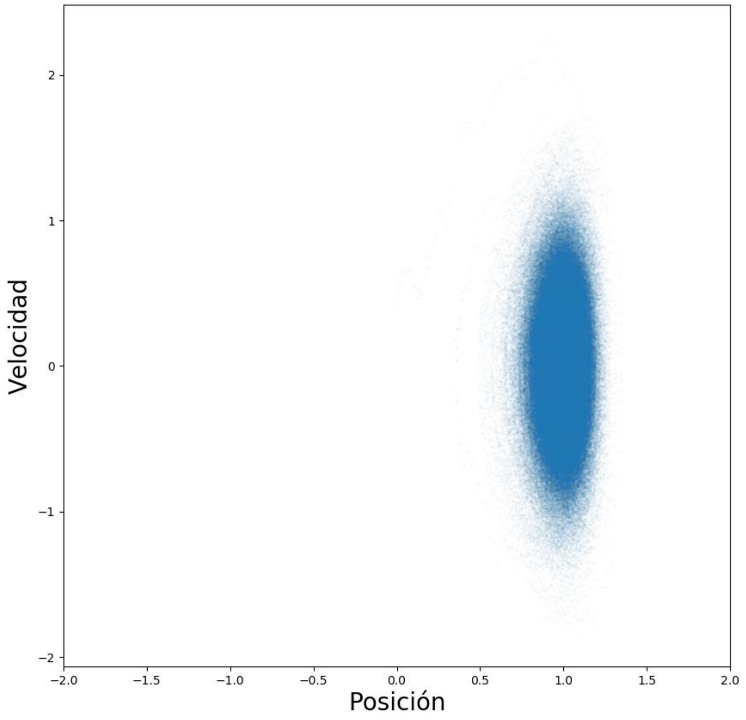
T=0.2 B=1
Eta=1



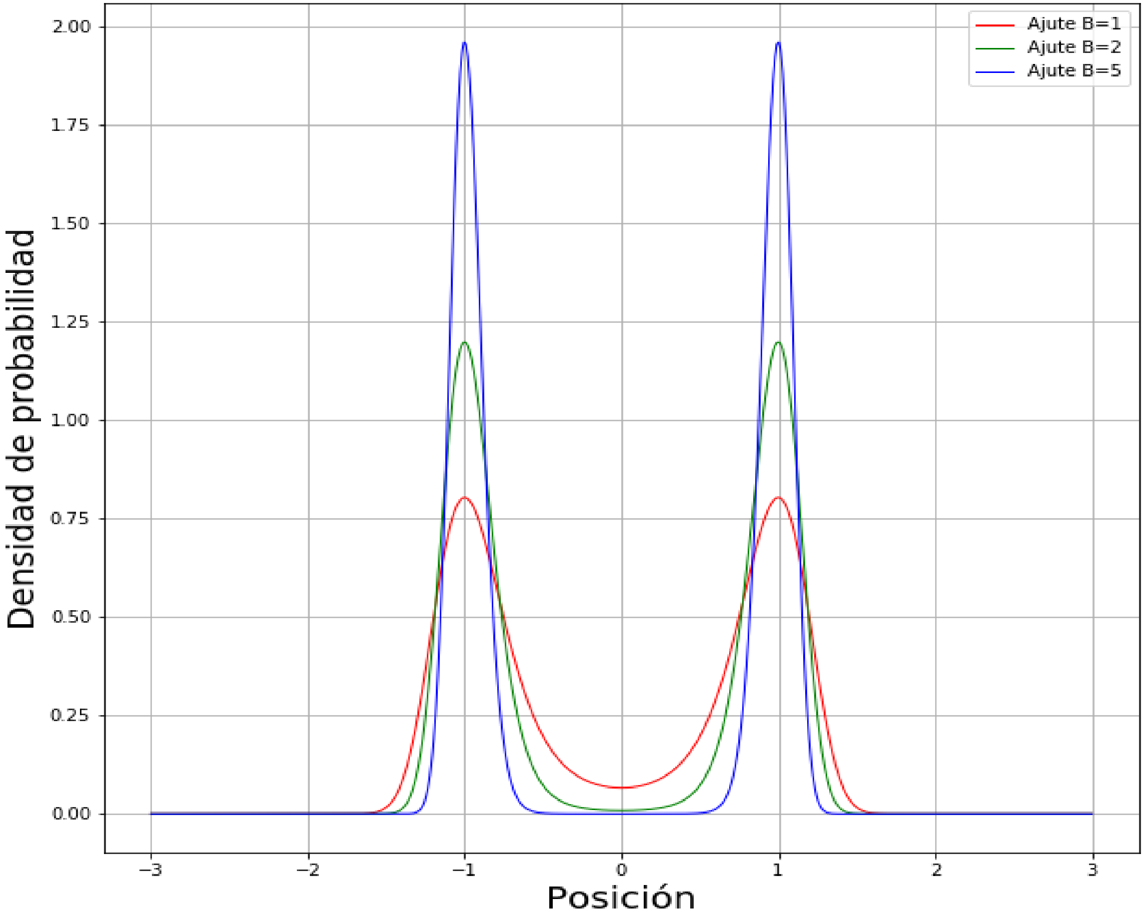
T=0.2 B=2
Eta=1



T=0.2 B=5
Eta=5



EVOLUCIÓN CON LA BARRERA



Ajuste
:

$$A \cdot e^{-V(x)/T}$$

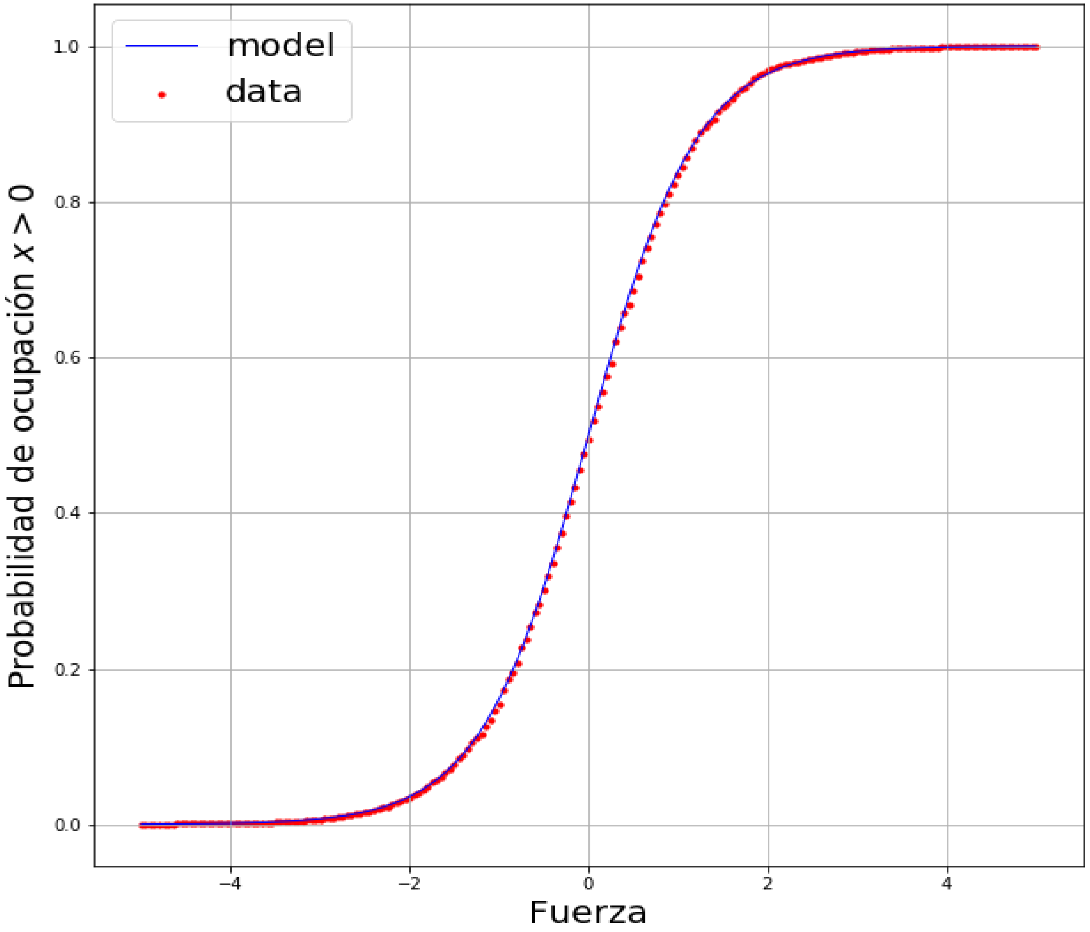
VARIACIÓN AL APLICAR FUERZA CTE

ECUACIÓN DEL MODELO

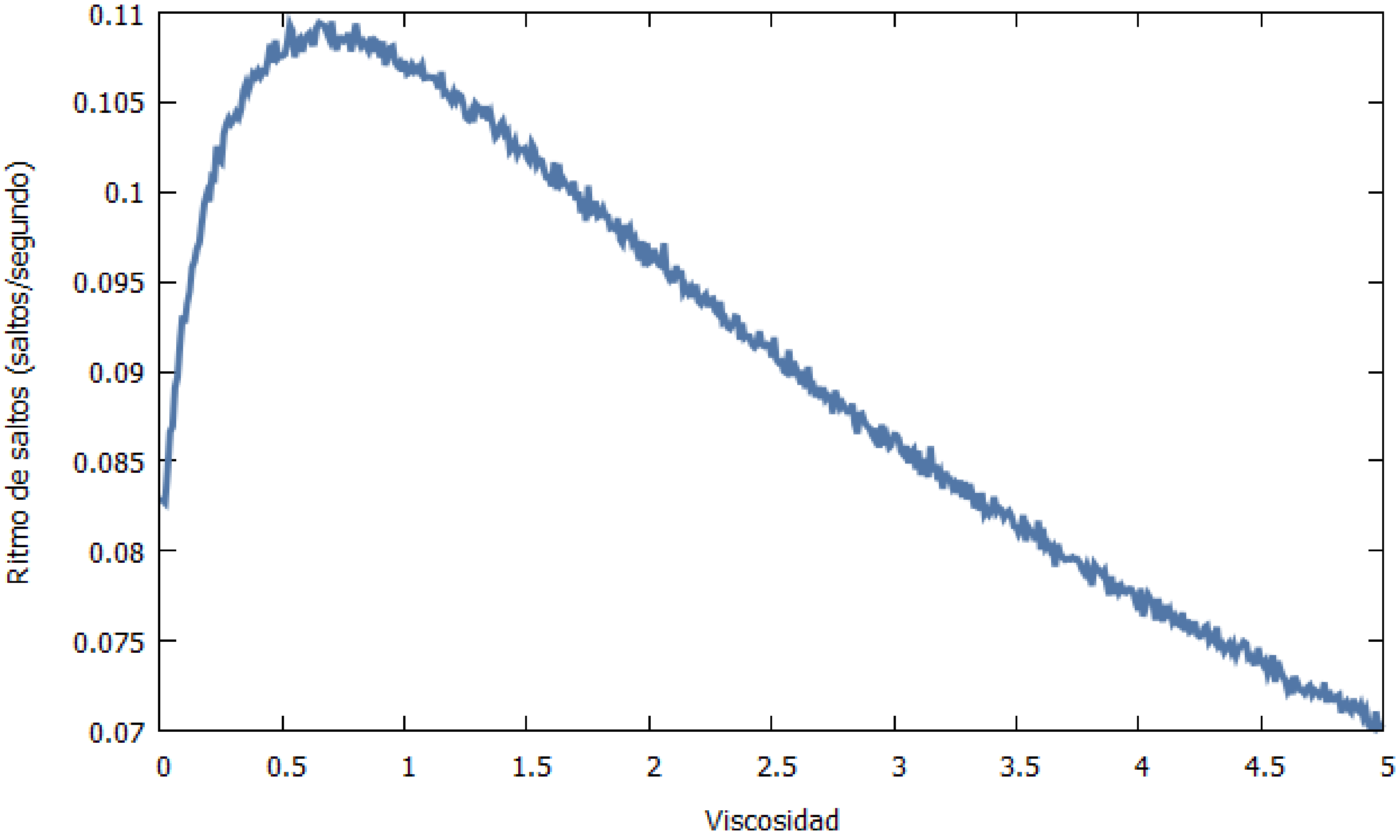
$$P(x) = \frac{1}{1 + e^{-\frac{F \cdot x}{T}}}$$

TEMPERATURA EFECTIVA

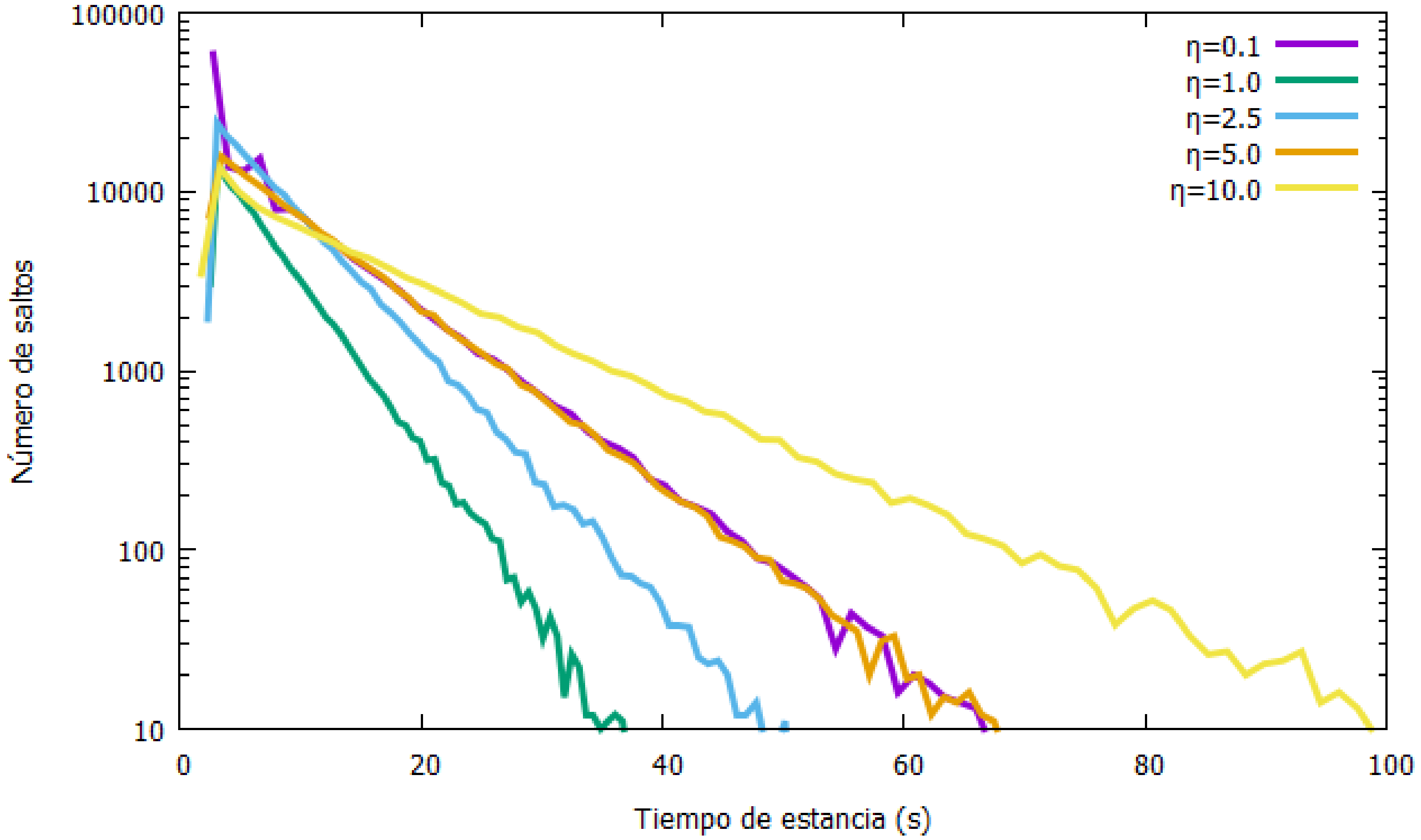
T=1.2



VARIACIÓN DEL RITMO DE CAMBIO CON LA VISCOSIDAD



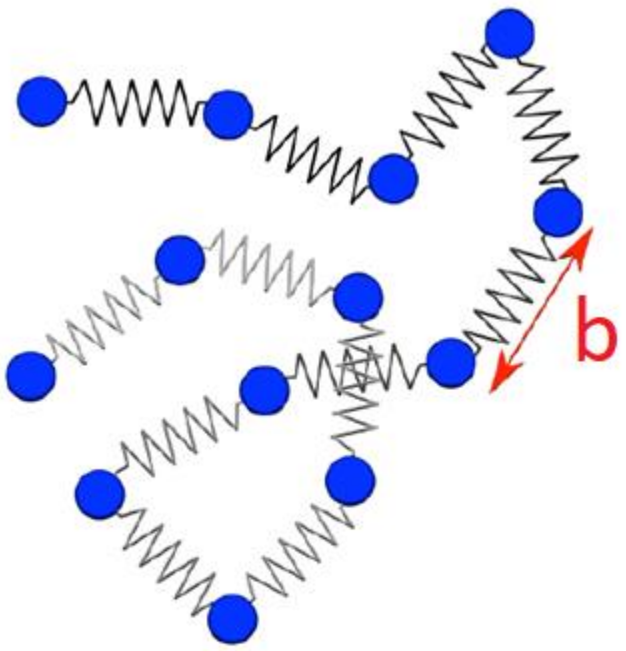
VARIACIÓN AL APLICAR FUERZA CTE

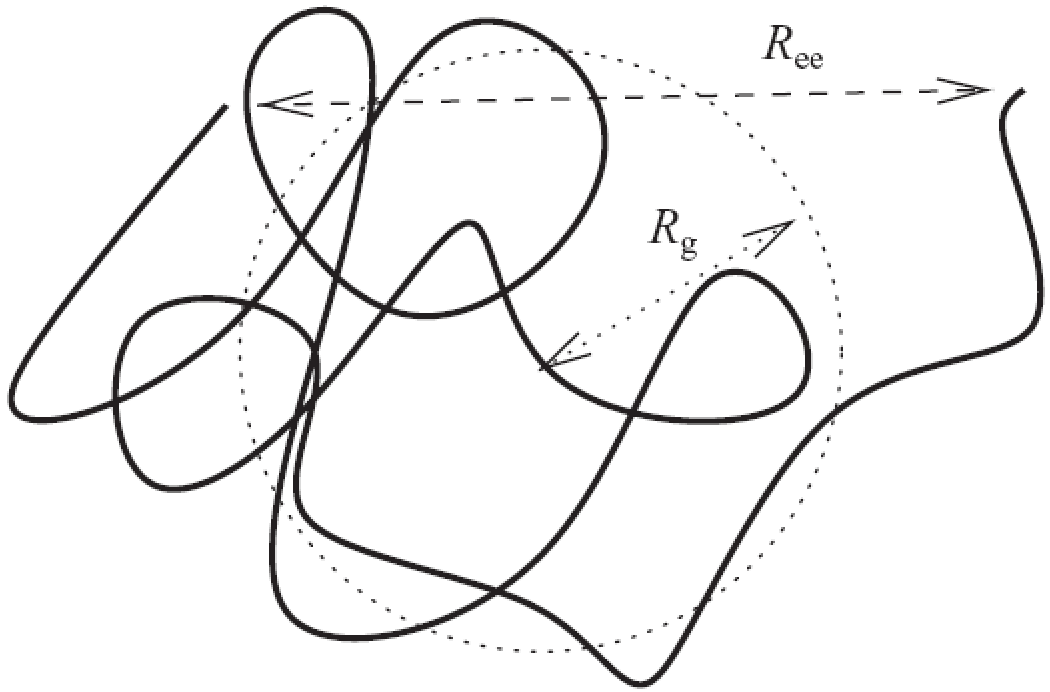


Modelo de polímero

$$V(\vec{r}_i, \vec{r}_{i+1}) = \frac{1}{2} k_e (|\vec{r}_i - \vec{r}_{i+1}| - b)^2$$

$$F(\vec{r}_i, \vec{r}_{i+1}) = k_e \left(1 - \frac{b}{|\vec{r}_i - \vec{r}_{i+1}|}\right)(x_{i+1} - x_i)$$

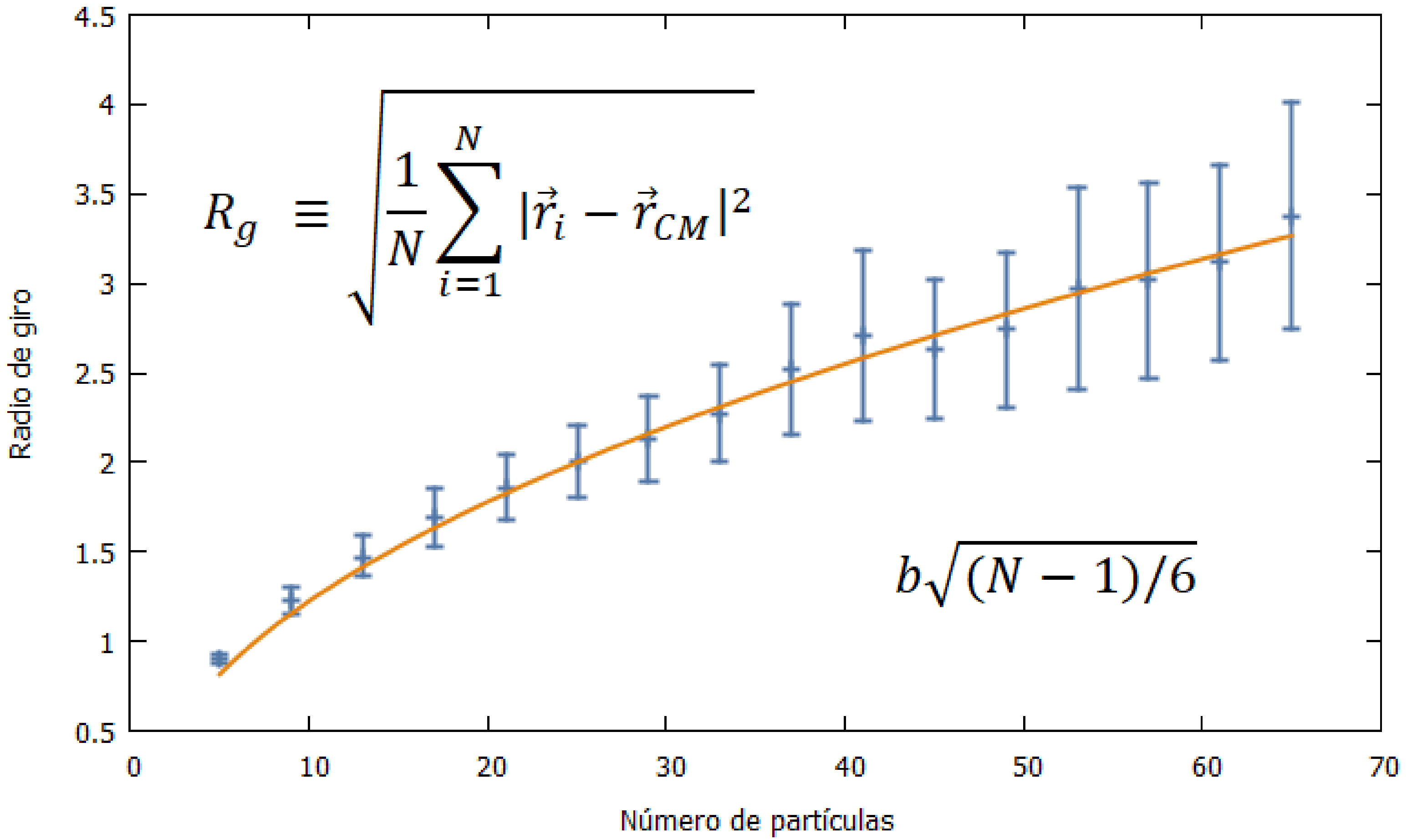




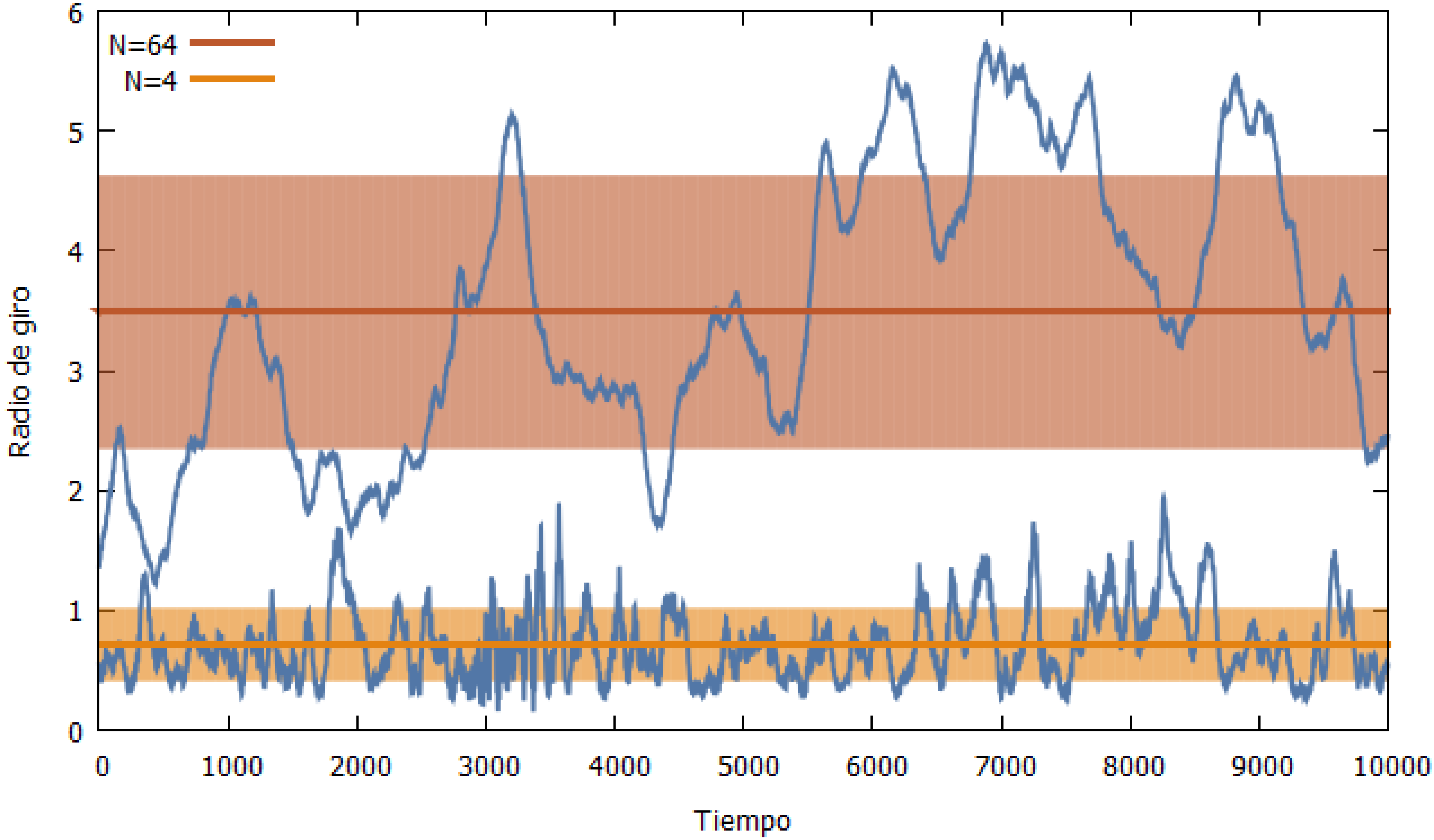
Equipartición (T=1)

Partículas	E. Cinética/muelle	E. Potencial/muelle
4	1.49	0.50
8	1.49	0.50
16	1.49	0.50
32	1.49	0.49
64	1.49	0.47

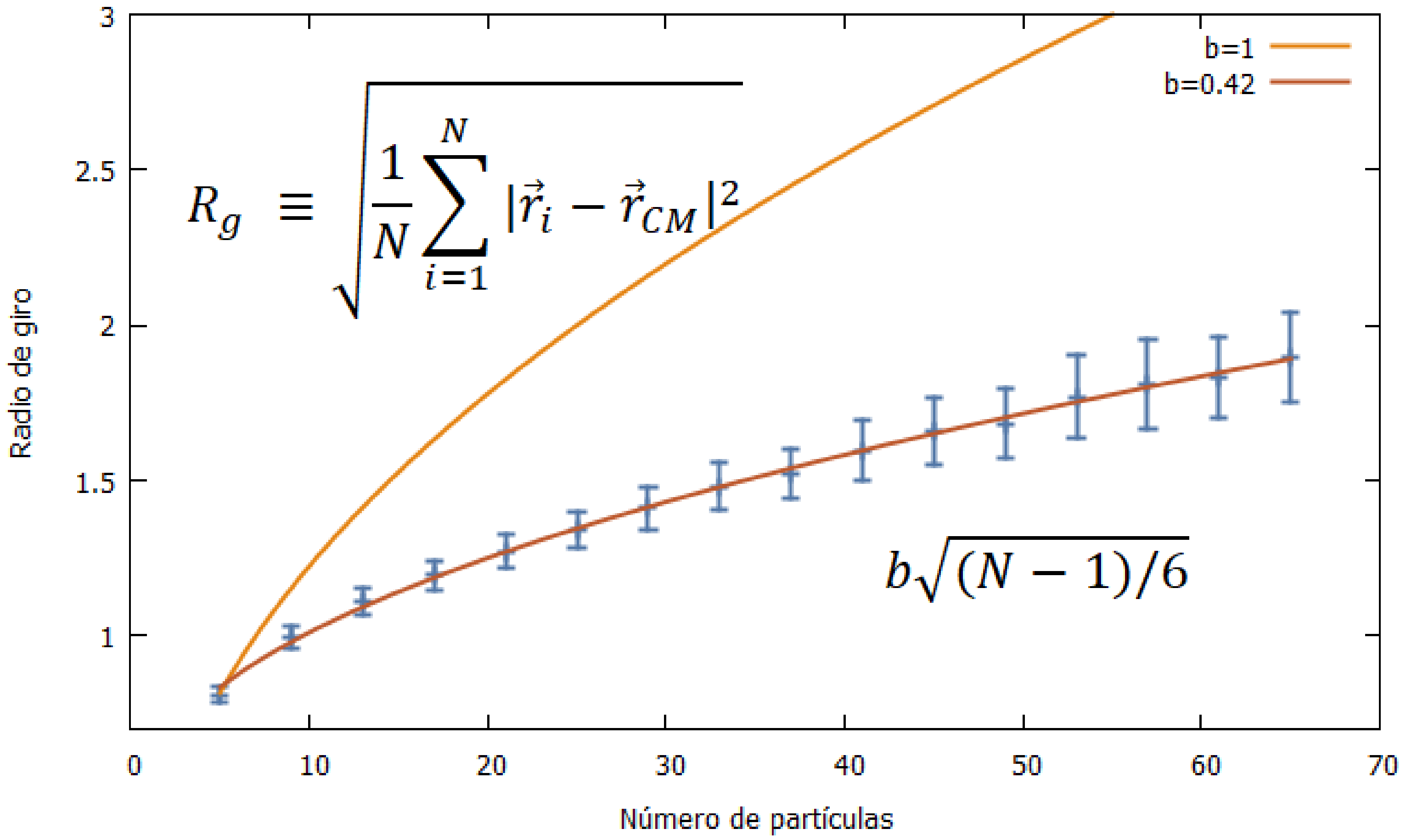
RADIO DE GIRO k_e=100



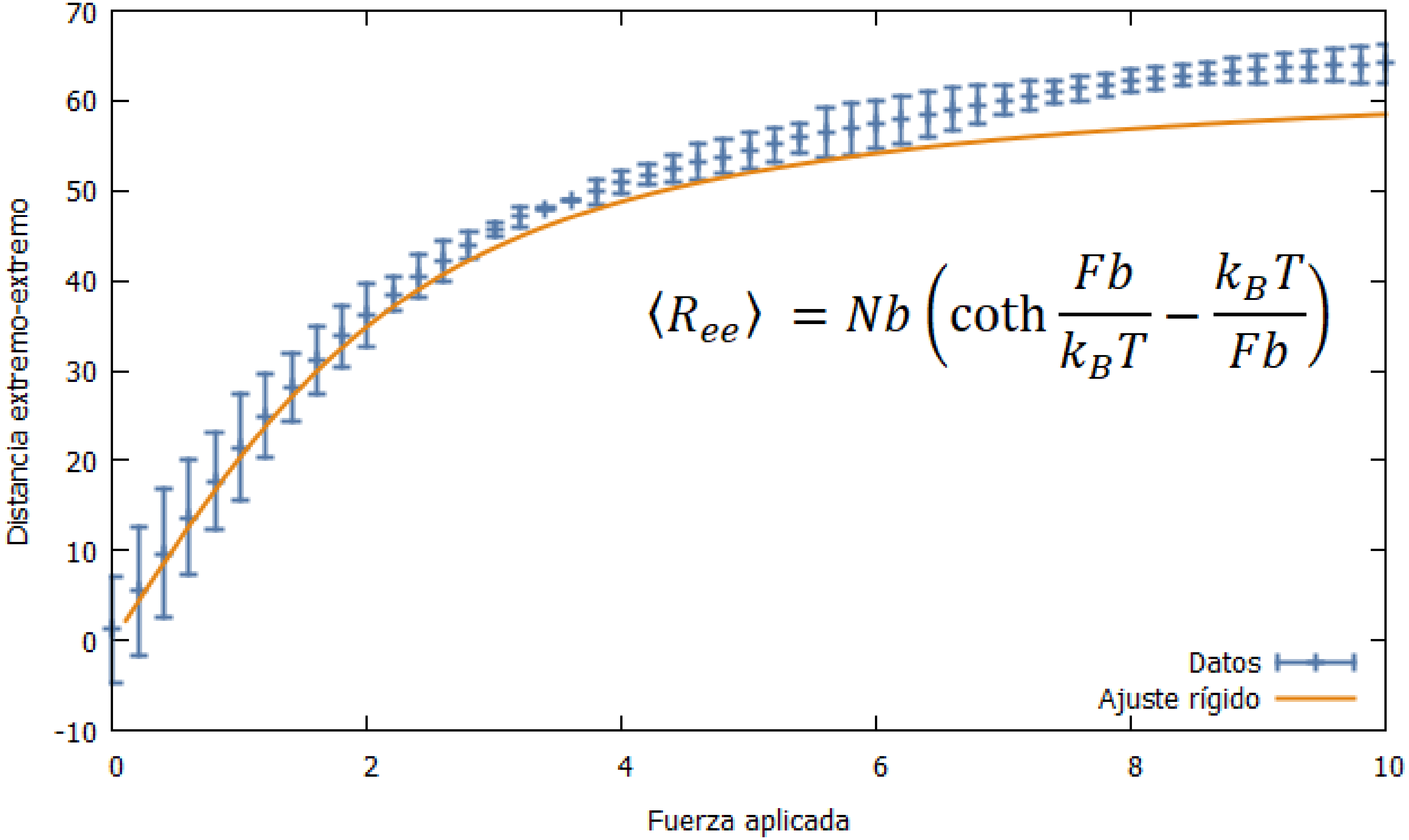
RADIO DE GIRO k_e=100



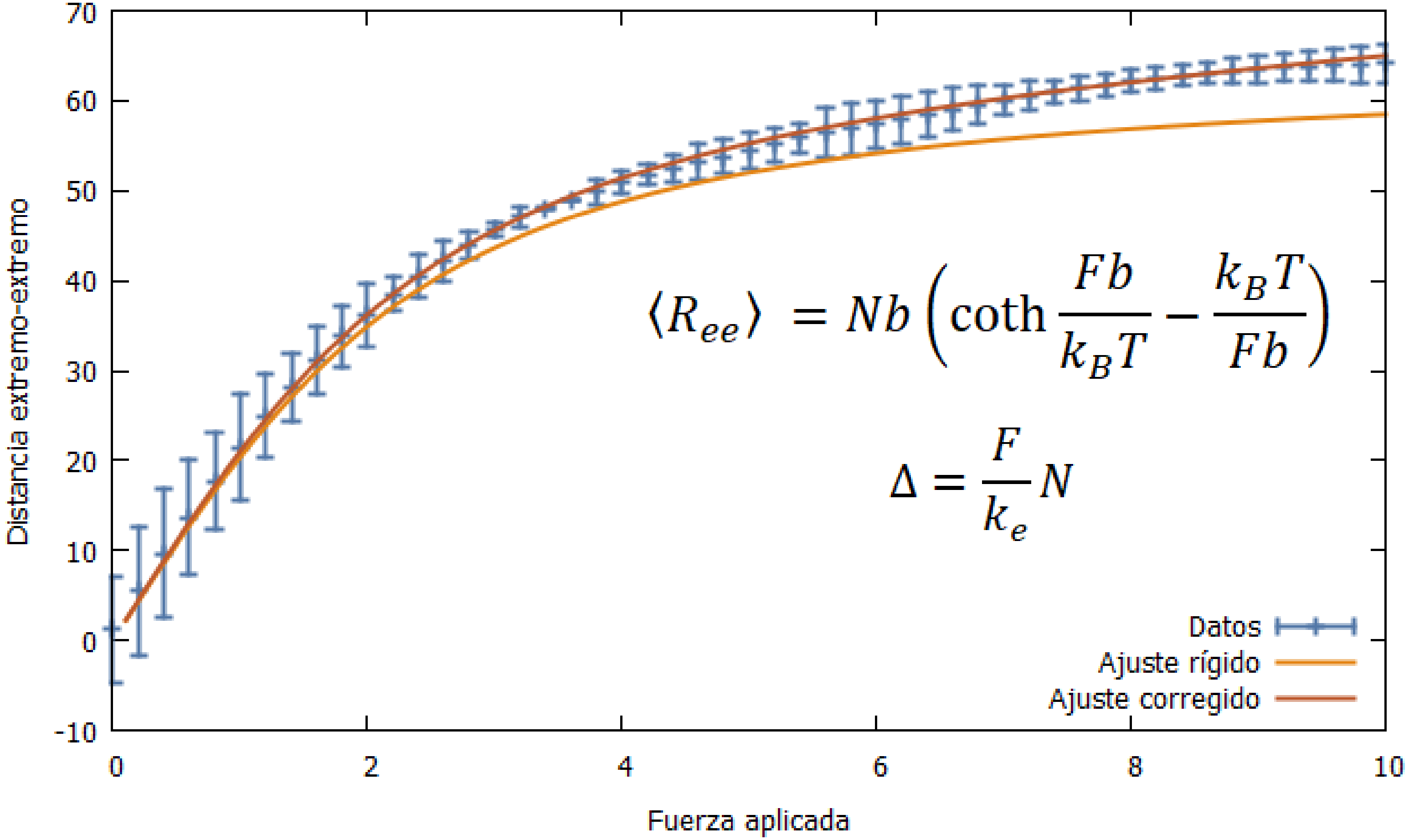
RADIO DE GIRO k_e=1000



Distancia de extremo a extremo (N=65, k=100)



Distancia de extremo a extremo (N=65 k_e=100)



Distancia de extremo a extremo (N=65 k_e=1000)