

Reporte de resultados de simulaciones

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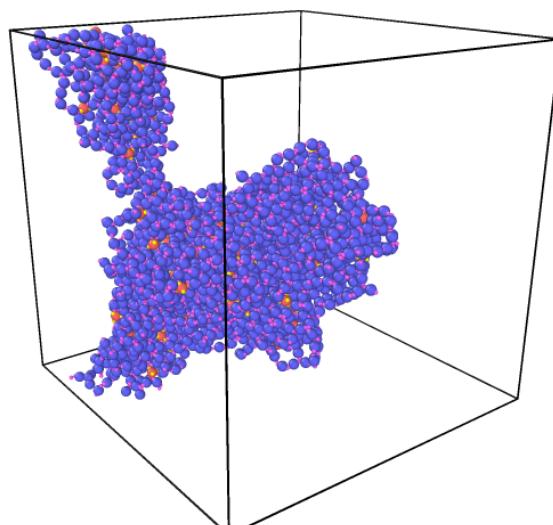
January 21, 2026

Documento en el que se muestran los análisis de las simulaciones realizadas en este directorio

Pruebas iniciales

Directory: o.050.30.052500-2026-01-16-102953

La simulación tardó, aproximadamente, 5 hrs. Fueron 2500 partículas y 8.5×10^6 iteraciones. Se asginó damp = 1 para ver que onda. Fracción de empaquetamiento y concentración de crosslinkers son irrelevantes por el momento.



- etotal = pe + ke
- ecouple = cumulative energy change due to thermo/baro
- econserve = pe + ke + ecouple
- ebond = bond energy
- eangle = angle energy
- emol = ebond + eangle + edihed + eimp

Figure 1: Configuración final del sistema. The econserve keyword is the sum of the potential and kinetic energy of the system as well as the energy that has been transferred by thermostating or barostating to their coupling reservoirs – that is, econserve = pe + ke + ecouple. Ideally, for a simulation in the NVT, NPH, or NPT ensembles, the econserve quantity should remain constant over time even though etotal may change.

El error proviene del archivo swapMech.3b. Estaba declarado de la siguiente forma:

```
PA PA PA 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PB PA PA 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PA PB PA 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PB PB PA 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PA PA PB 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PB PA PB 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PA PB PB 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PB PB PB 0.6 swapMechTab1_w0.75.table SEC1 linear 100
```

La diferencia con el archivo swapMechTab2_w0.75.table es la evaluación de los potenciales. En el archivo 1 tiene más elementos evaluados que en el segundo archivo. Esto por la forma que tiene LAMMPS para evaluar potenciales numéricos¹.

¹... There are two different cases. If element 2 and element 3 are of the same type (e.g. SiCC),... If element 2 and element 3 are not of the same type (e.g. SiCSi),... Therefore, the total number of table entries is "M = N * N * (N+1)" for the symmetric (element 2 and element 3 are of the same type) and "M = 2 * N * N * N" for the general case (element 2 and element 3 are not of the same type).

Directory: 0.050.30.05500-2026-01-20-111704

Main fix:

```
PA PA PA 0.6 swapMechTab2_w0.75.table SEC1 linear 100
PB PA PA 0.6 swapMechTab2_w0.75.table SEC1 linear 100
PA PB PA 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PB PB PA 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PA PA PB 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PB PA PB 0.6 swapMechTab1_w0.75.table SEC1 linear 100
PA PB PB 0.6 swapMechTab2_w0.75.table SEC1 linear 100
PB PB PB 0.6 swapMechTab2_w0.75.table SEC1 linear 100
```

Ahora, el problema principal es la aglomeración de interacción de más de dos patches, se tiene que $w = 0.75$,

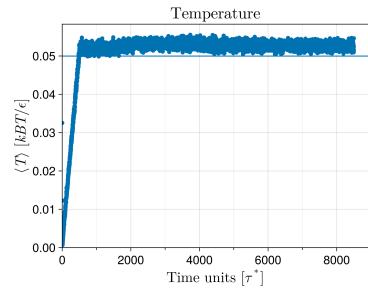
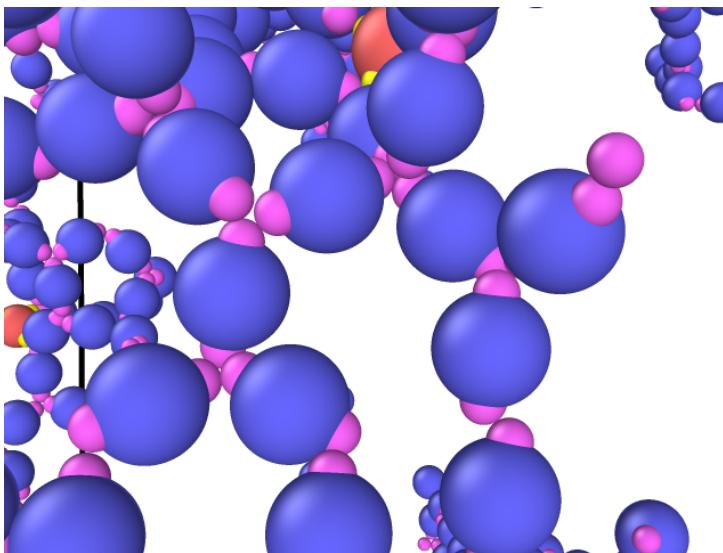


Figure 2: Temperature during assembly.

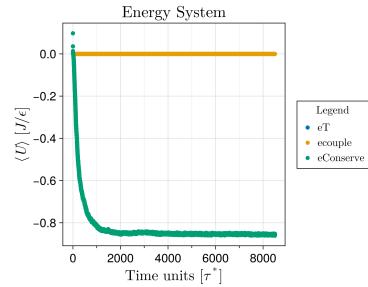


Figure 3: Econserve and ecouple.

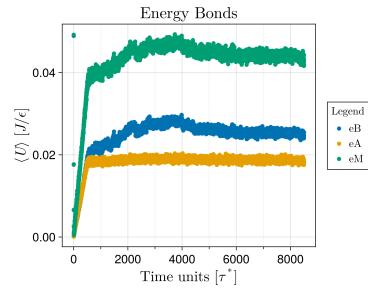


Figure 4: Bonds de la partícula patchy

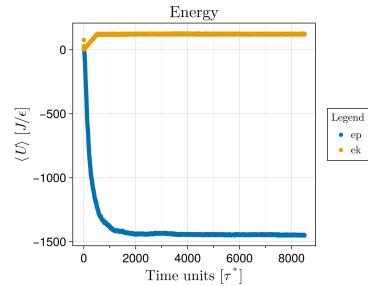
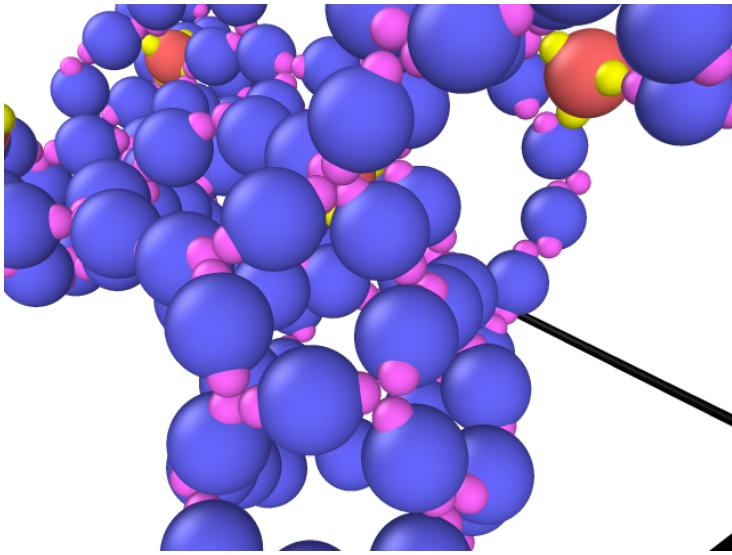


Figure 5: ep y ek

Directory: 0.050.30.05500-2026-01-20-121005

En esta simulación se cambió el parámetro w a $w = 1$,



Parece que incrementar el parámetro w , incrementa la cantidad de interacciones entre patches. Posiblemente sea error de signo en la evaluación de la fuerza o potencial, porque debería de pasar lo contrario, por la definición del potencial.

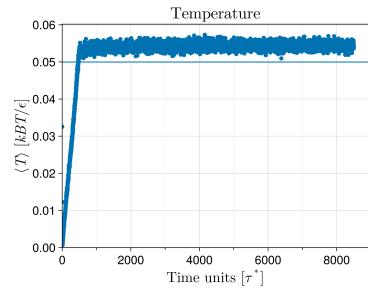


Figure 6: Temperature during assembly.

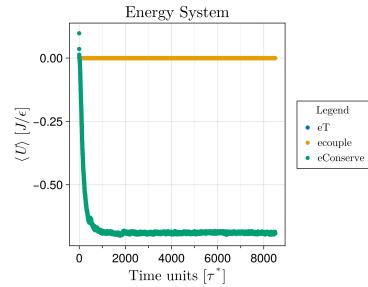


Figure 7: Econserve and ecouple.

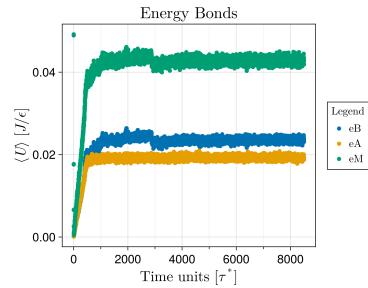


Figure 8: Bonds de la partícula patchy

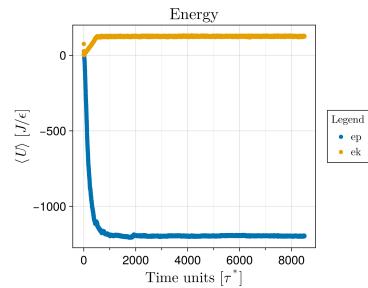


Figure 9: ep y ek

Directory: 0.050.30.05500-2026-01-20-135923

$w = 2$ Para reducir el tiempo de espera, la cantidad de iteraciones se disminuyeron a 5.5×10^6 . Se tardó 36 minutos.

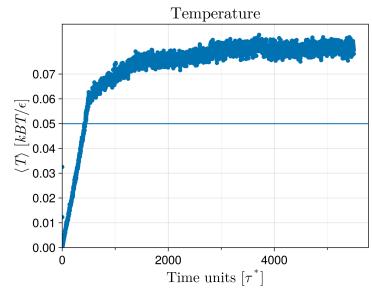
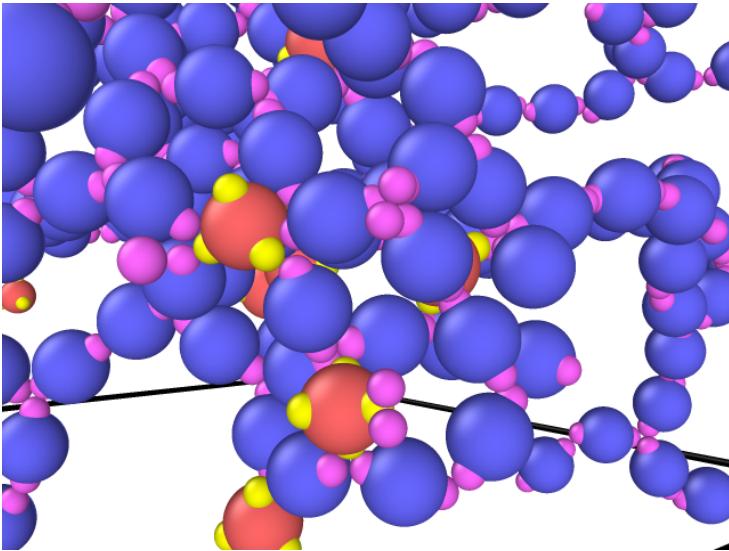


Figure 10: Temperature during assembly.

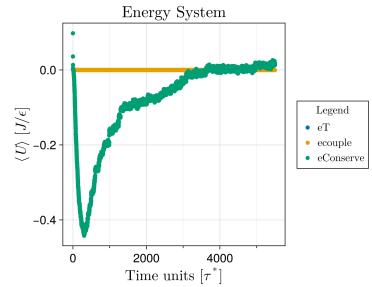


Figure 11: Econserve and ecouple.

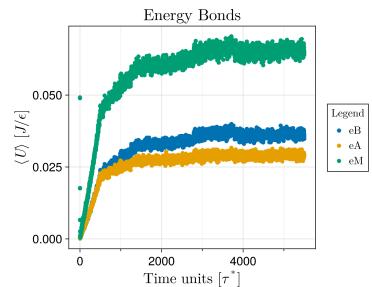


Figure 12: Bonds de la partícula patchy

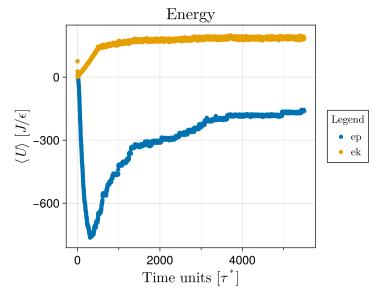
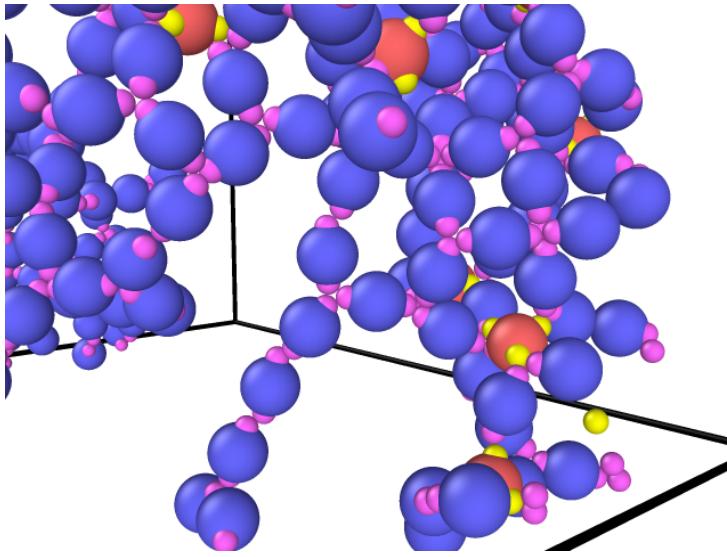


Figure 13: ep y ek

Directory: 0.050.30.05500-2026-01-20-143651

Ahora se explora con $w = 0.5$ 35 minutos.



Mi intuición ahora es que puede que tenga mal las diferencias finitas. En las simulaciones que use para la Tesis de maestría se tenía el $damp = 0.1$ y ahora es de $damp = 1$. Intuyo que también por eso no se está logrando estabilizar mucho esto. También, viendo rápidamente la temperatura, está se relaja arriba de 0.05, lo cuál no es esperado.

Volveré a intentar, pero cambiaré la masa de las partículas patchy a 1, a ver que onda.

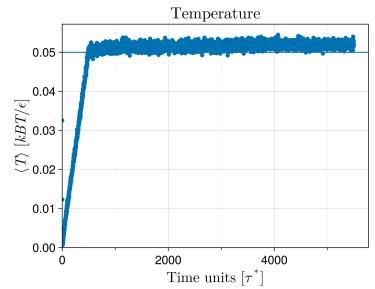


Figure 14: Temperature during assembly.

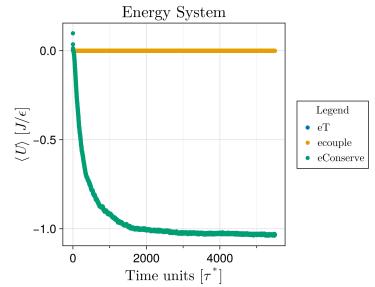


Figure 15: Econservate and ecouple.

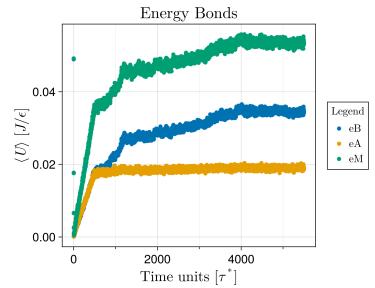


Figure 16: Bonds de la partícula patchy

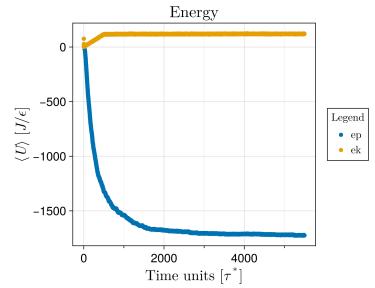
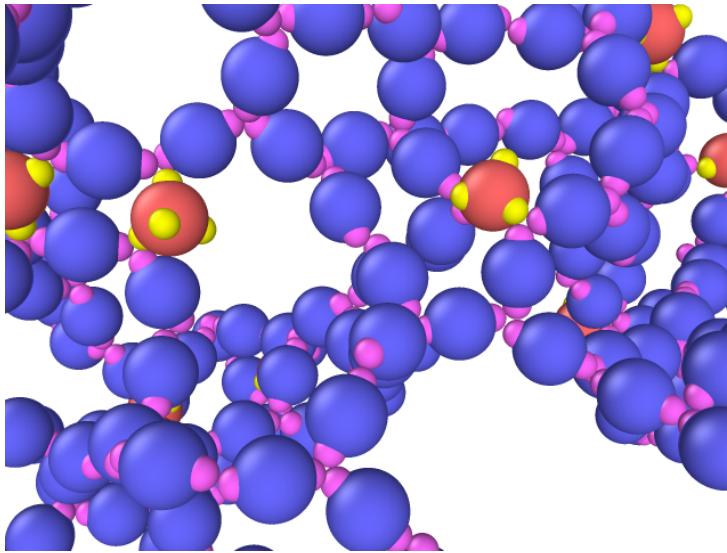


Figure 17: ep y ek

Directory: 0.050.30.05500-2026-01-20-151755

Ahora se explora con $w = 1$ Masa de partículas patchy de 0.1 a 1. 32 minutos.



No se ‘‘arreglo’’ la interacción de más de dos patches, pero parece ser que la temperatura si se estabilizó en el valor esperado, 0.05.

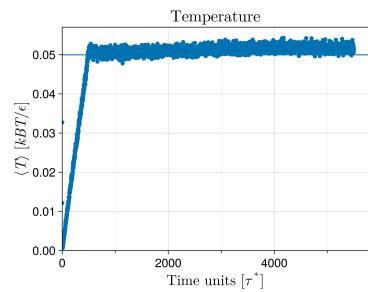


Figure 18: Temperature during assembly.

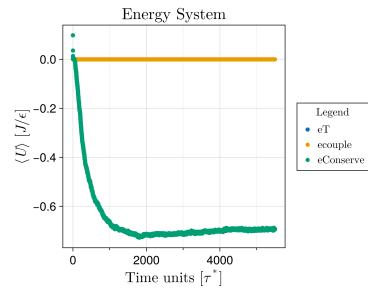


Figure 19: Econserve and ecouple.

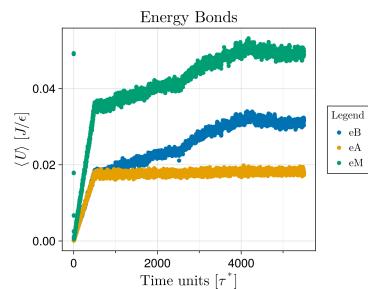


Figure 20: Bonds de la partícula patchy

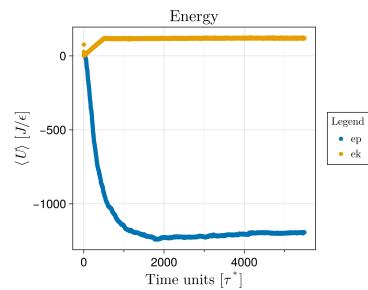


Figure 21: ep y ek

Directory: 0.050.30.05500-2026-01-21-133721

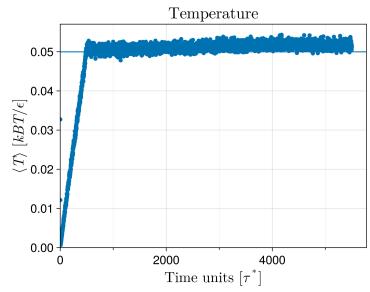


Figure 22: Temperature during assembly.

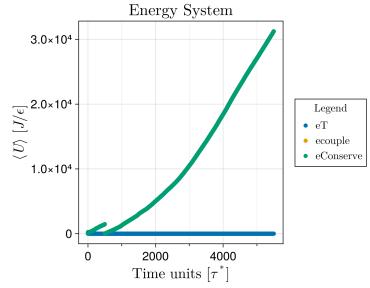


Figure 23: Econserve and ecouple.

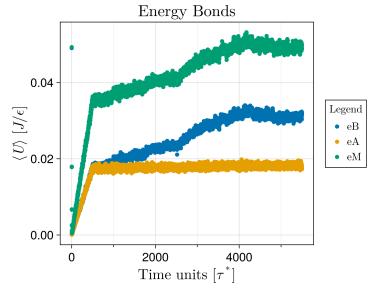


Figure 24: Bonds de la partícula patchy

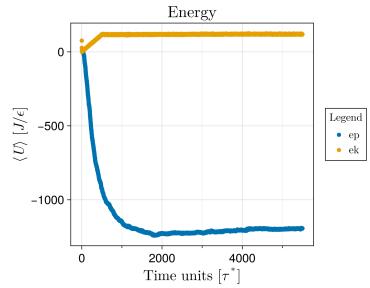


Figure 25: ep y ek