

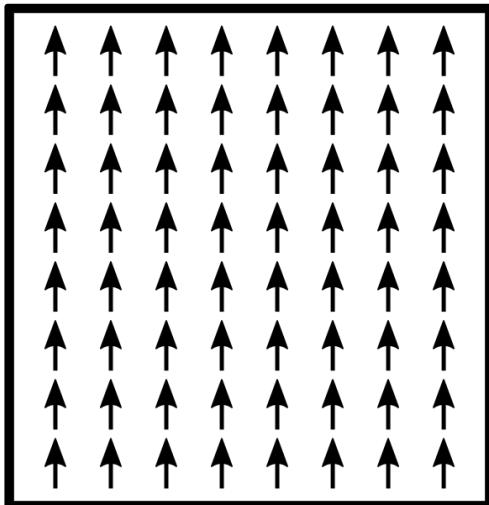
# Simulación de sistemas magnéticos por medio del método Monte Carlo

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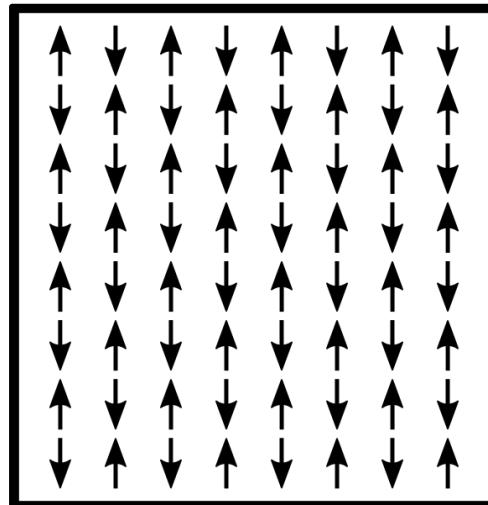
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2. Aspectos generales
3. Método Monte Carlo
4. Algoritmo de Metropolis
5. Algoritmo Adaptativo
6. Vegas
7. Ejemplos

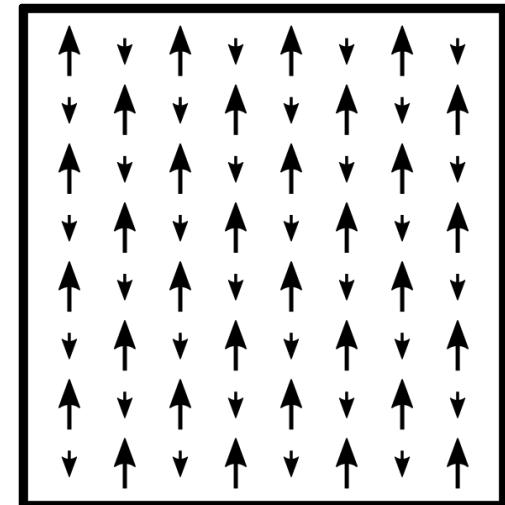
# Fundamentación teórica



Ferromagnético  
(FM)

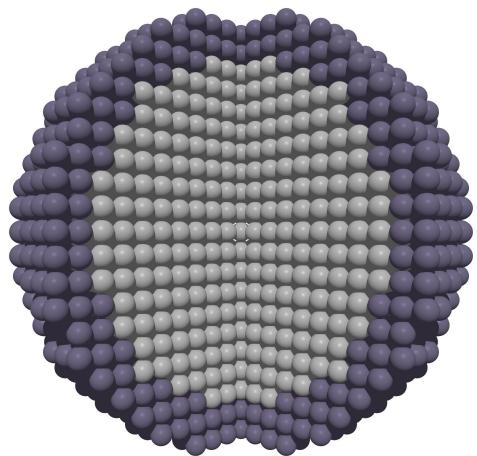


Antiferromagnético  
(AFM)

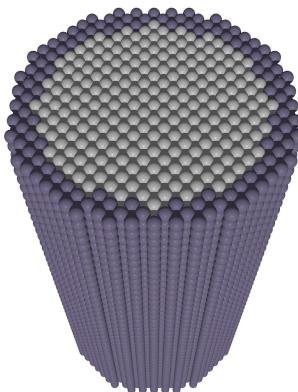


Ferrimagnético  
(FiM)

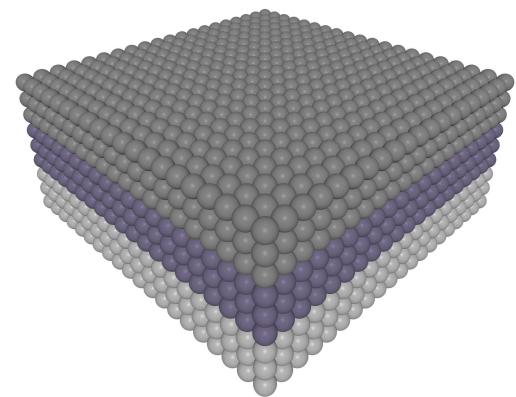
# Nanoestructuras magnéticas



Nanopartícula  
*core/shell*



Nanohilo  
*core/shell*

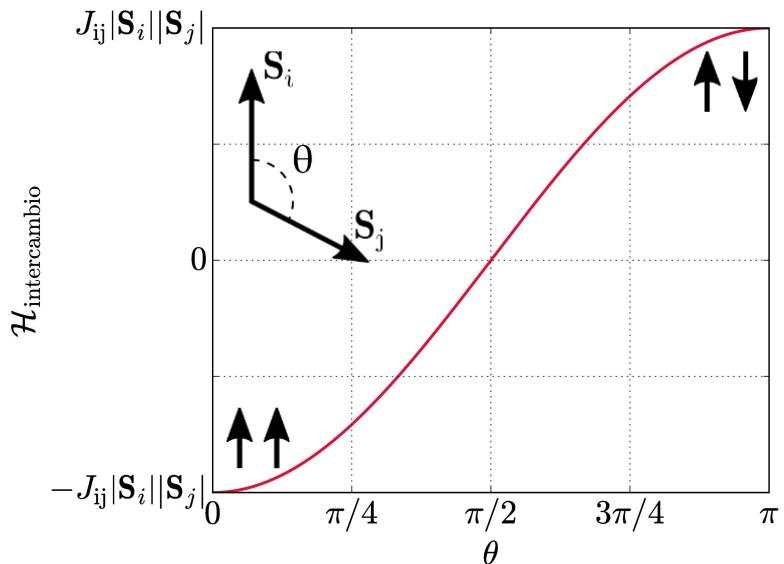


Multicapas

# Términos energéticos

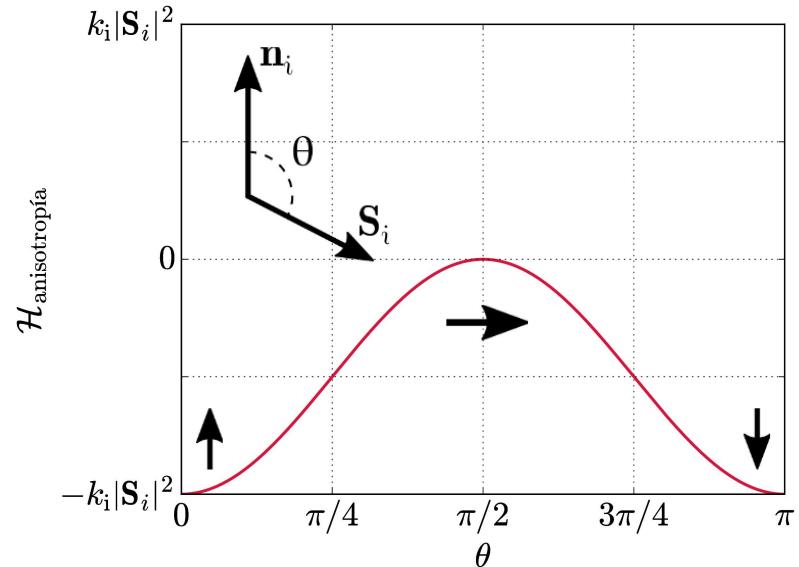
## Intercambio magnético

$$\mathcal{H}_{\text{intercambio}} = - \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$



## Anisotropía magnetocristalina

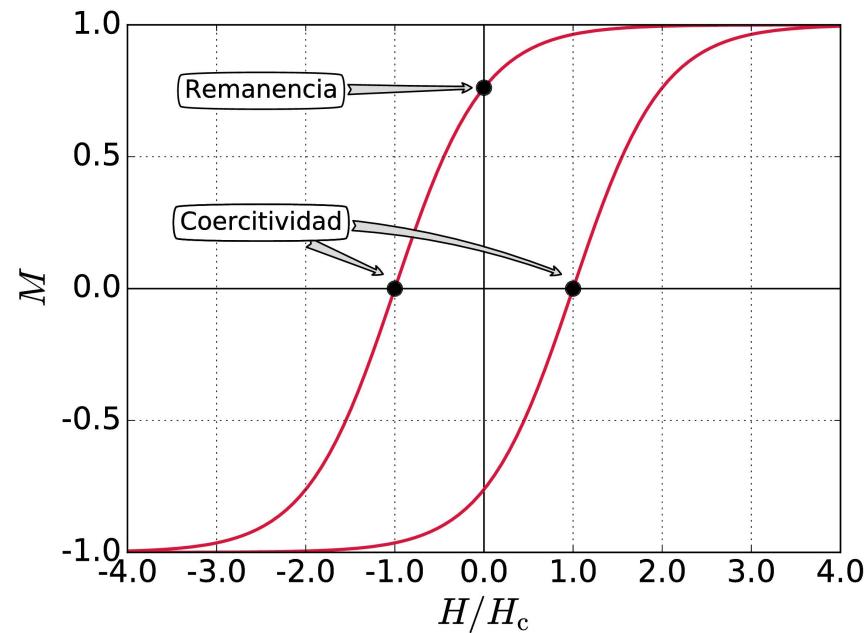
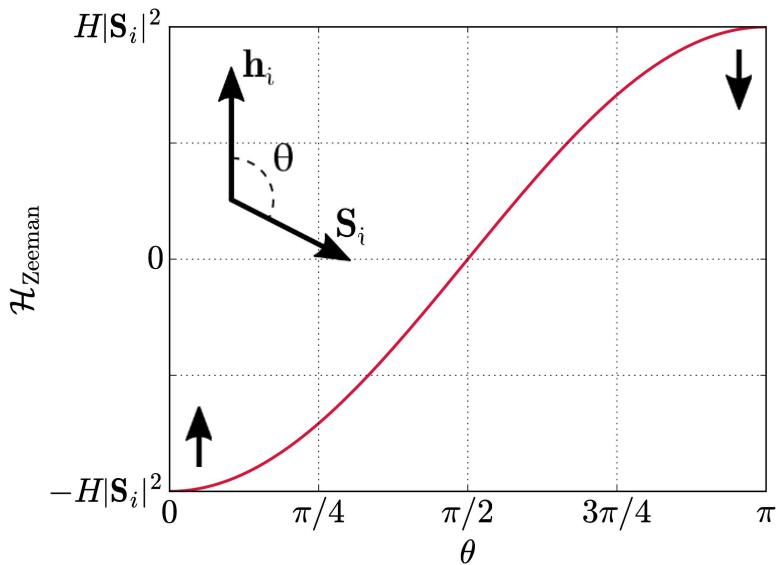
$$\mathcal{H}_{\text{anisotropia}} = - \sum_i k_i (\mathbf{S}_i \cdot \mathbf{n}_i)^2$$



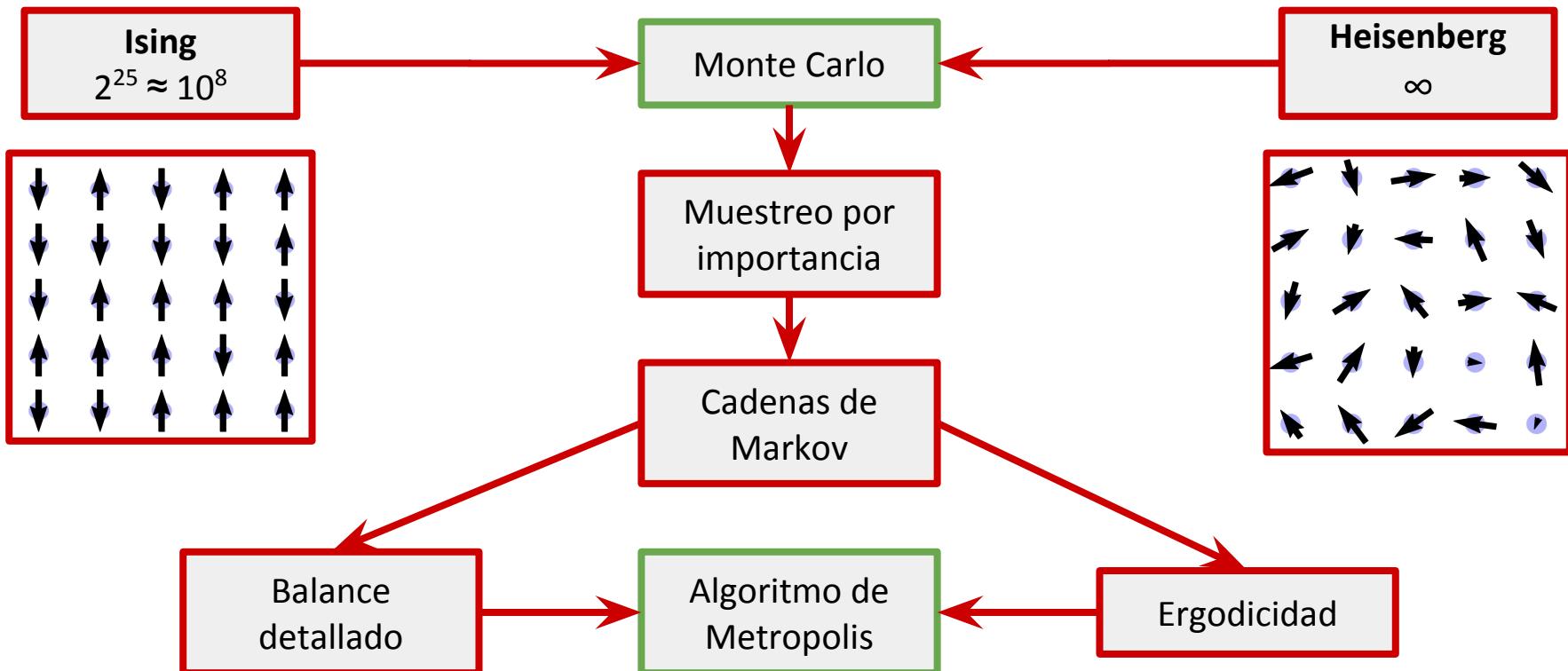
# Términos energéticos

Influencia de un campo externo

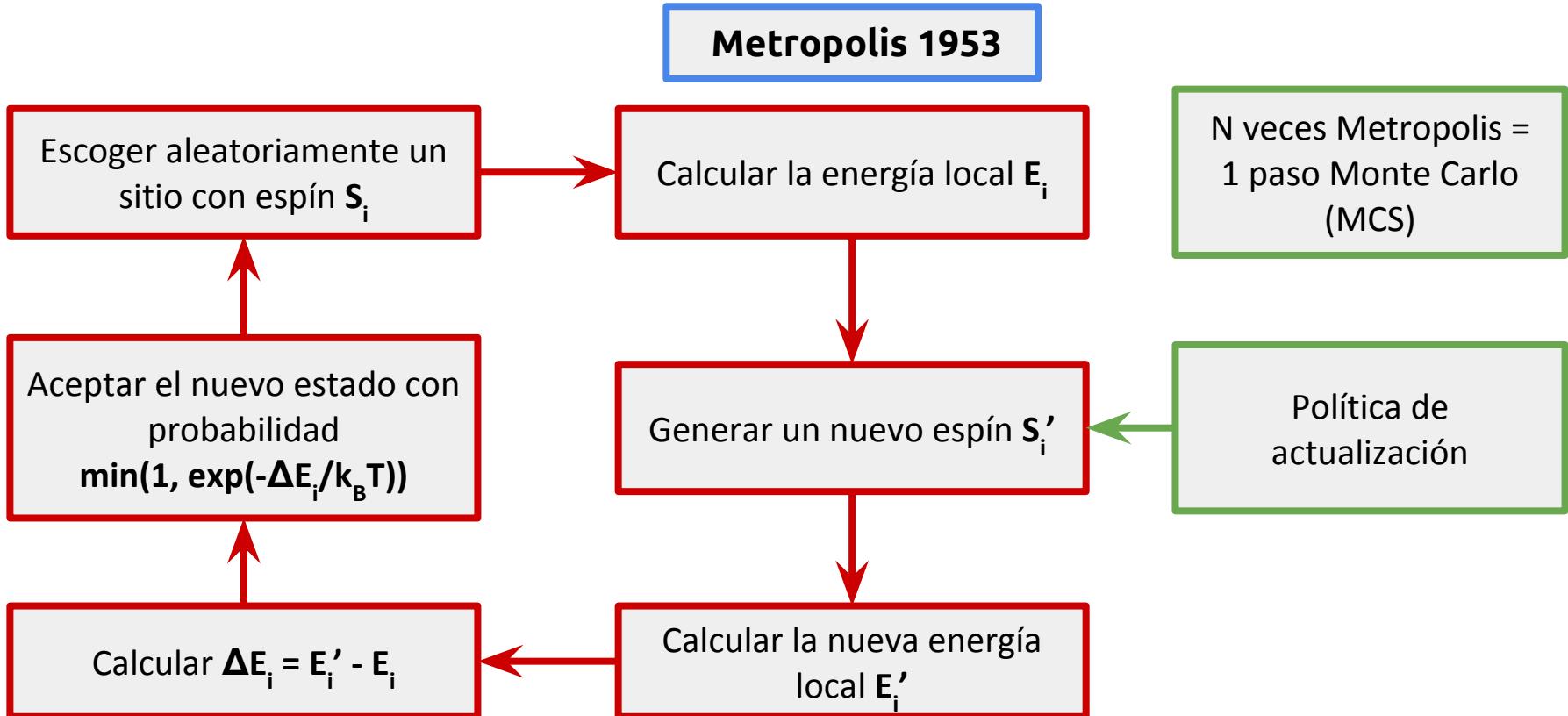
$$\mathcal{H}_{\text{Zeeman}} = -H \sum_i \mu_i \mathbf{S}_i \cdot \mathbf{h}_i$$



# Método Monte Carlo

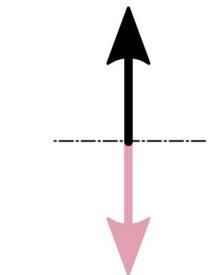


# Algoritmo de Metropolis

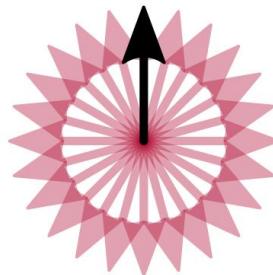


# Políticas de actualización

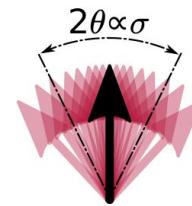
Spin flip



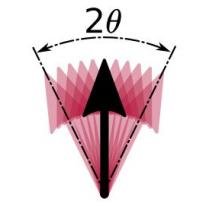
Aleatoria



Gaussiana



Small step



$$S'_i = -S_i$$

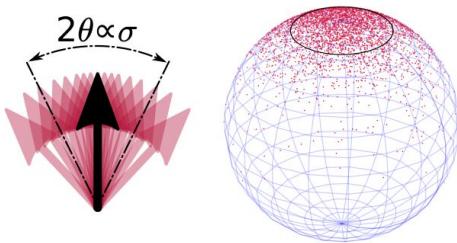
$$S'_i = \frac{\Gamma}{|\Gamma|}$$

$$S'_i = \frac{S_i + \sigma \Gamma}{|S_i + \sigma \Gamma|}$$

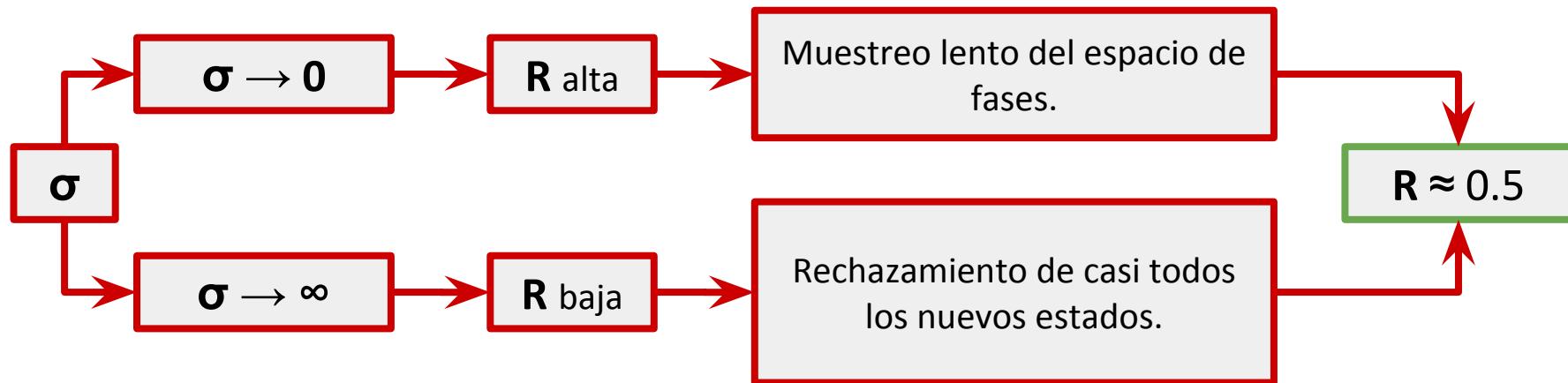
# Algoritmo Adaptativo

Gaussiana

$$S'_i = \frac{S_i + \sigma \Gamma}{|S_i + \sigma \Gamma|}$$



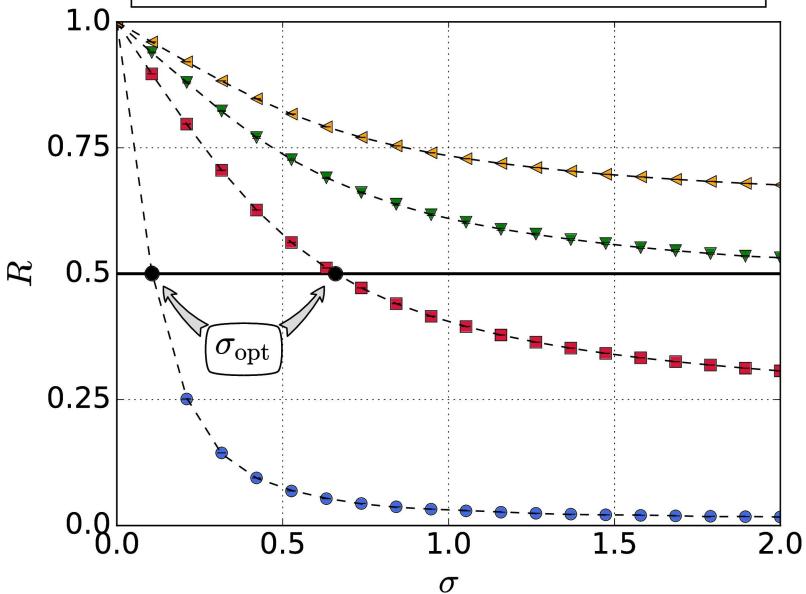
Tasa de aceptación:  
 $R = R(\sigma, \Delta E, T)$



# Algoritmo Adaptativo

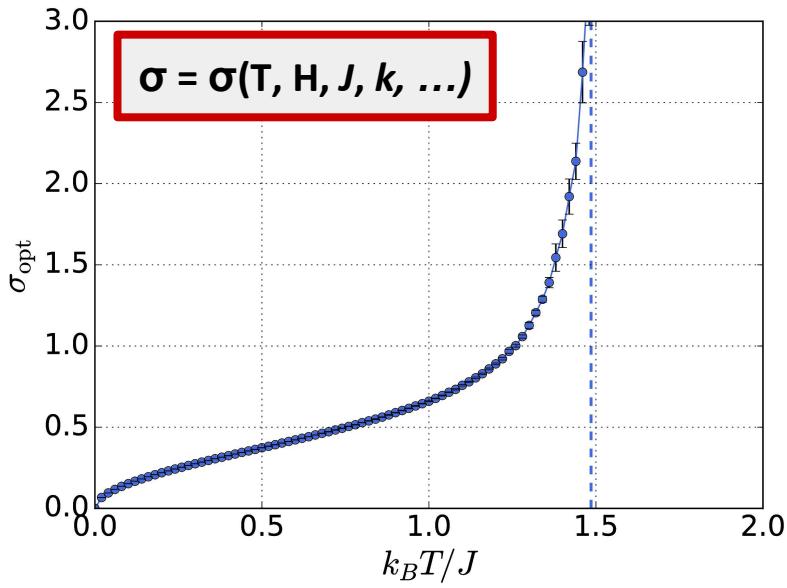
$$\mathcal{H} = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - k \sum_i (\mathbf{S}_i \cdot \mathbf{u}_z)^2 - H \sum_i (\mathbf{S}_i \cdot \mathbf{u}_z)$$

<span style="color: blue;">●</span>	<span style="color: blue;">●</span>	$k_B T/J = 0.05$	<span style="color: green;">▼</span>	<span style="color: green;">▼</span>	$k_B T/J = 1.48$
<span style="color: red;">■</span>	<span style="color: red;">■</span>	$k_B T/J = 1.0$	<span style="color: orange;">△</span>	<span style="color: orange;">△</span>	$k_B T/J = 2.0$

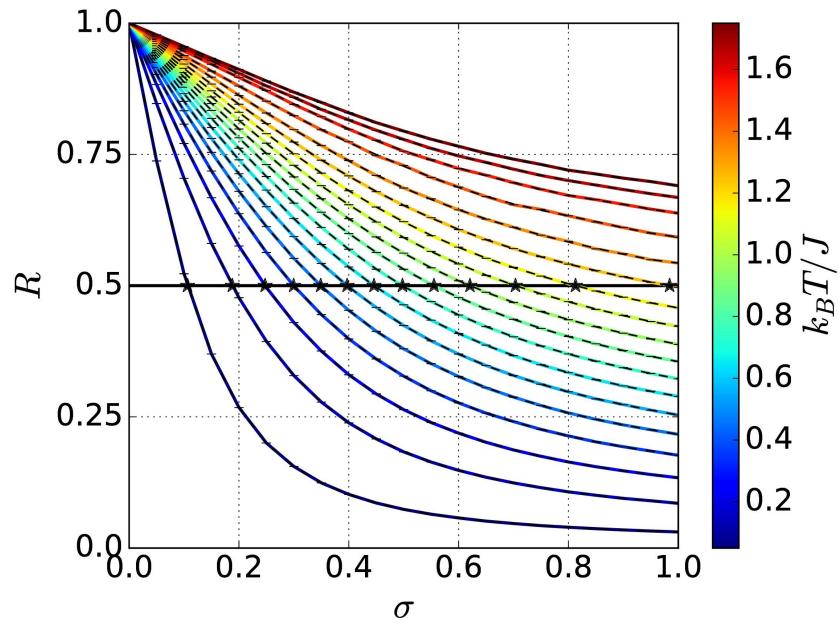


$$\begin{aligned} J &= 1.0 \\ k &= 0.001J \end{aligned}$$

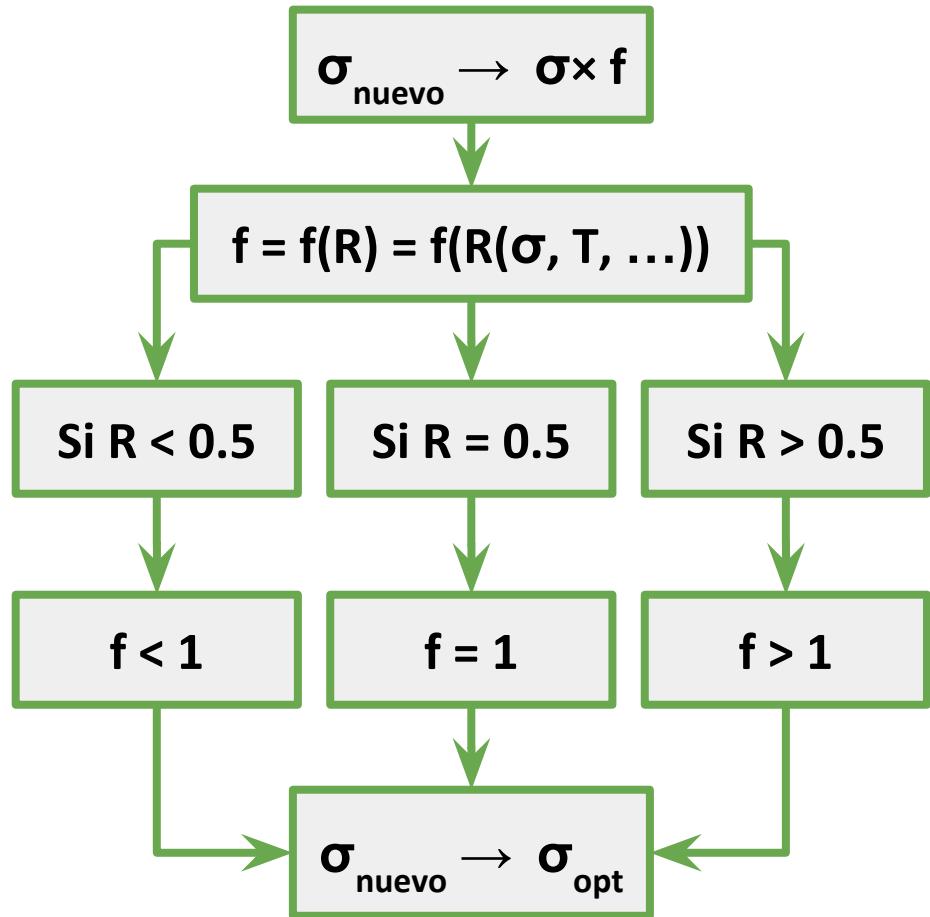
$$\frac{k_B T_C}{J} = 1.485427$$



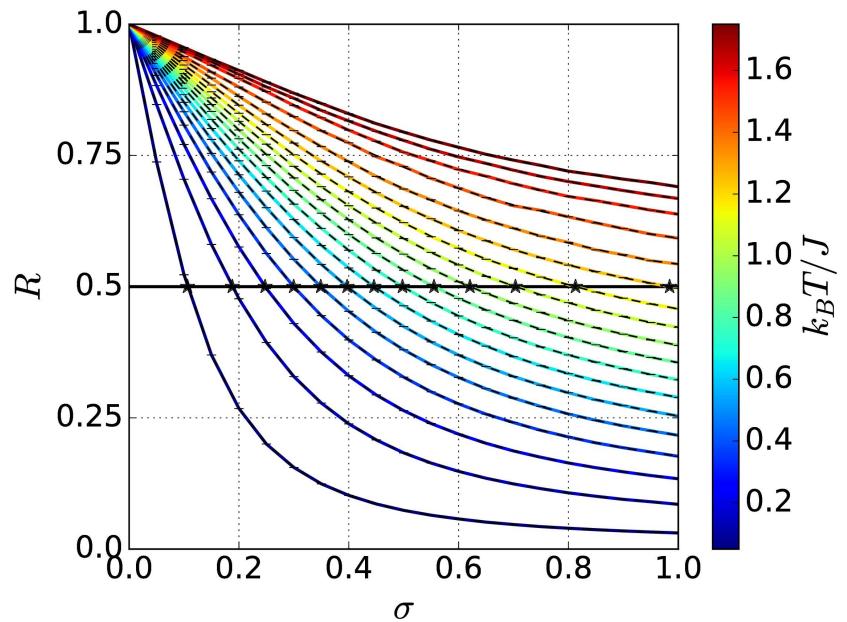
# Algoritmo Adaptativo



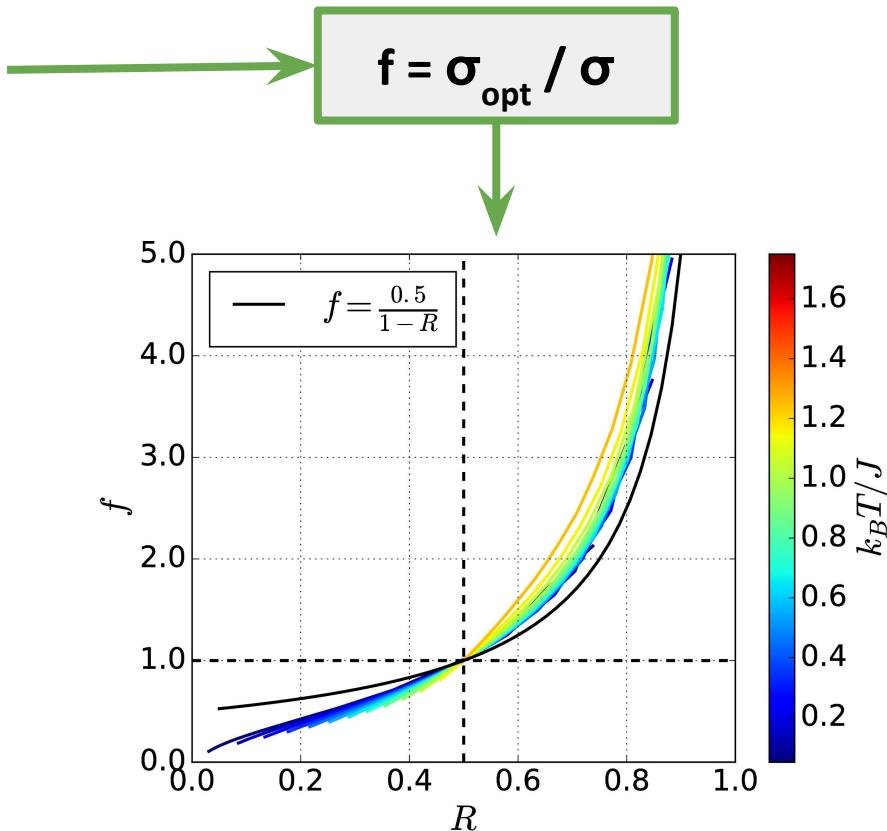
$$\frac{k_B T_C}{J} = 1.485427$$



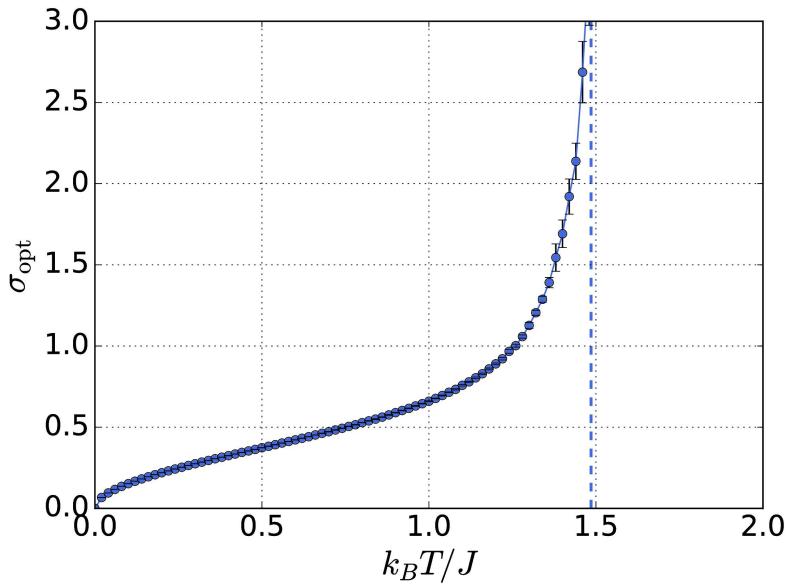
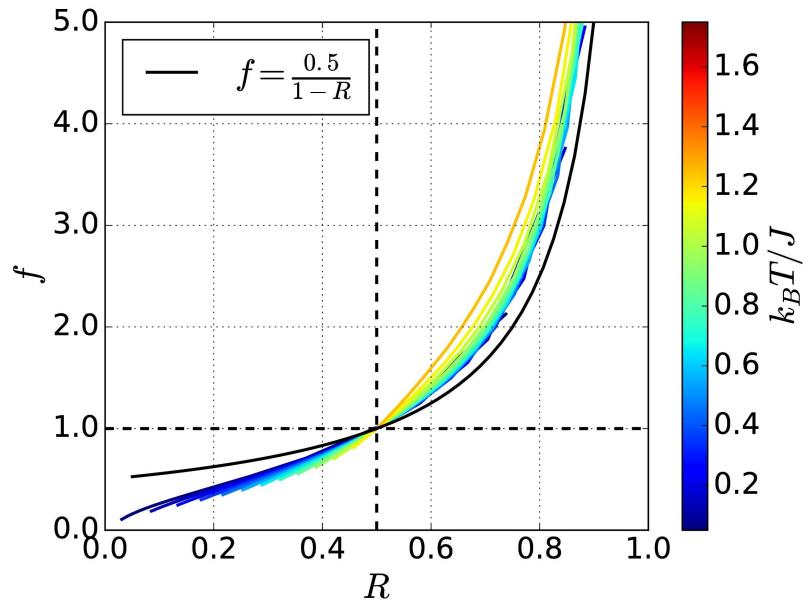
# Algoritmo Adaptativo



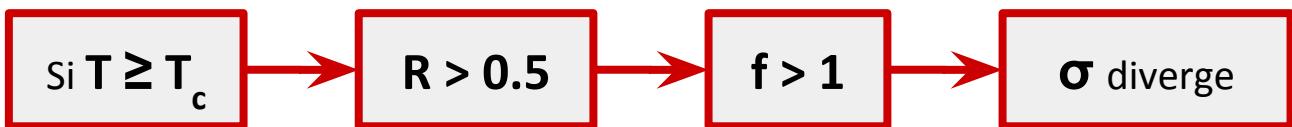
$$\frac{k_B T_C}{J} = 1.485427$$



# Algoritmo Adaptativo



$$\frac{k_B T_C}{J} = 1.485427$$

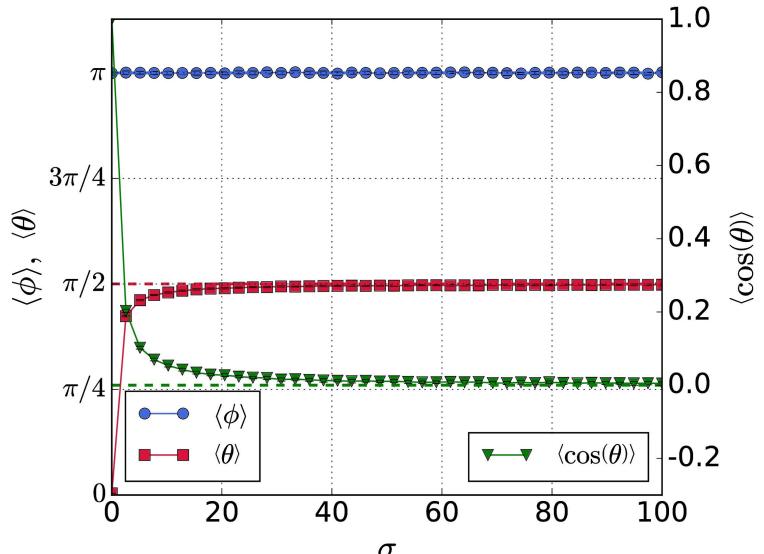


# Algoritmo Adaptativo

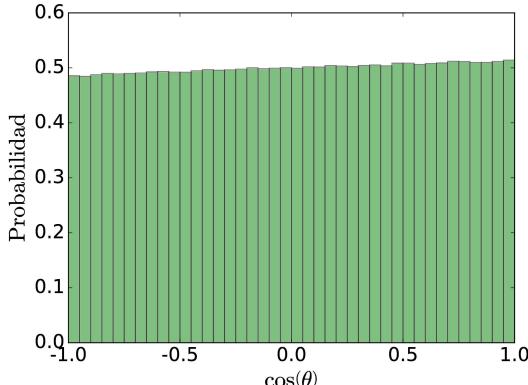
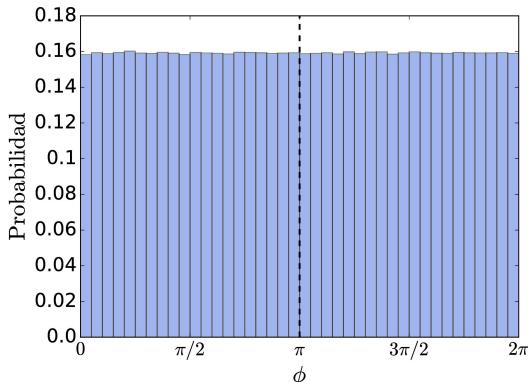
Gaussiana

$$S'_i = \frac{S_i + \sigma \Gamma}{|S_i + \sigma \Gamma|} \xrightarrow{\sigma \rightarrow \infty} S'_i = \frac{\Gamma}{|\Gamma|}$$

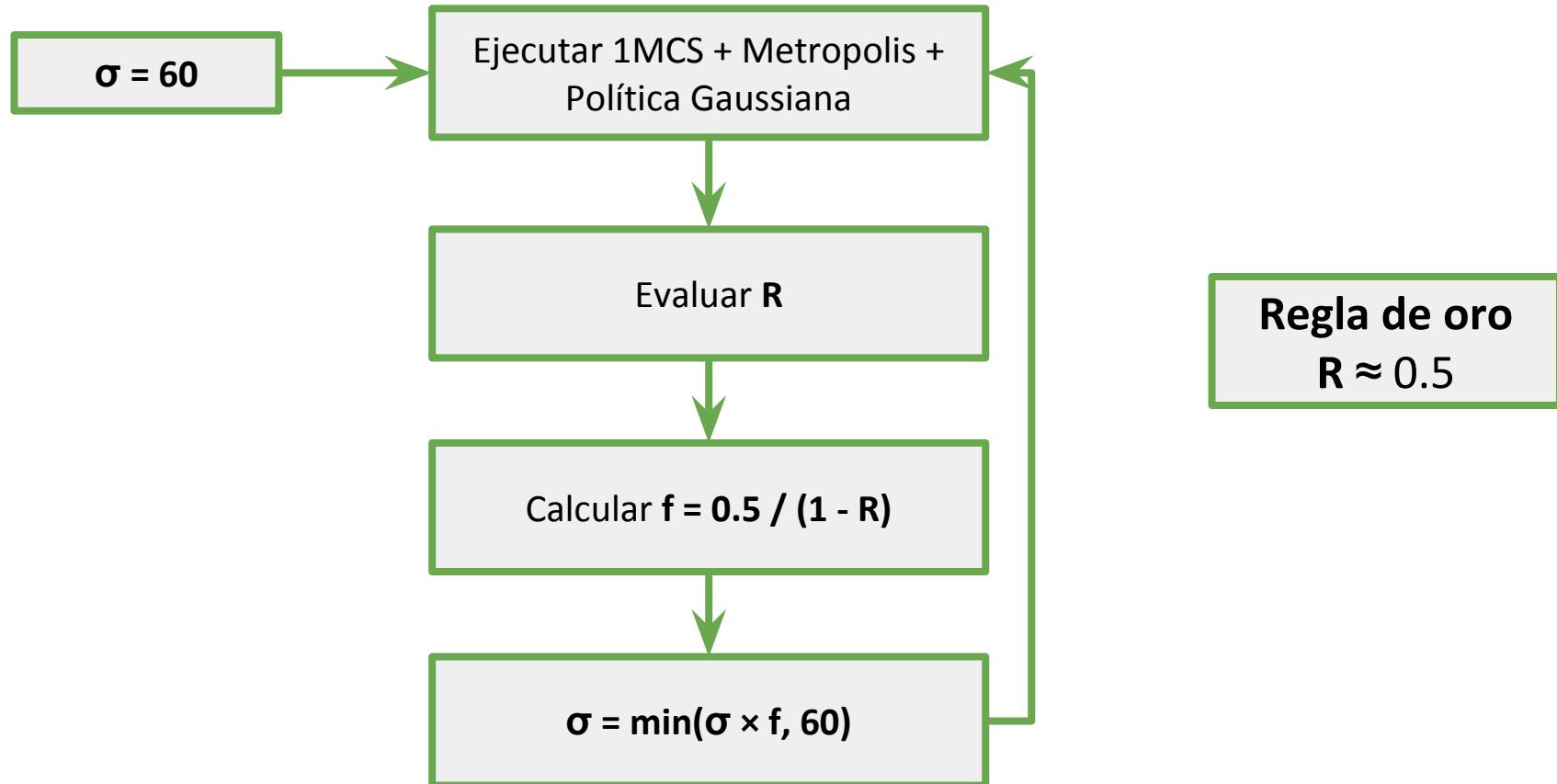
Aleatoria



$\sigma_{\text{máx}} = 60$



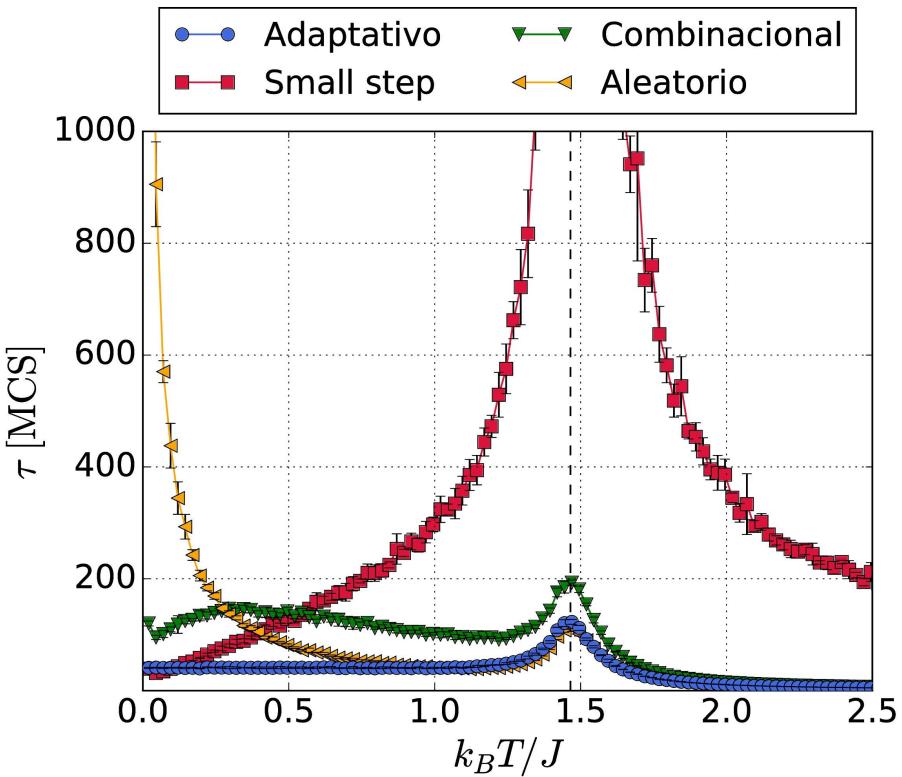
# Algoritmo Adaptativo



**Regla de oro**  
 $R \approx 0.5$

# Algoritmo Adaptativo

Tiempos de correlación



Adaptativo es hasta 20 veces mejor que Aleatorio

# Vegas

Algoritmo Adaptativo



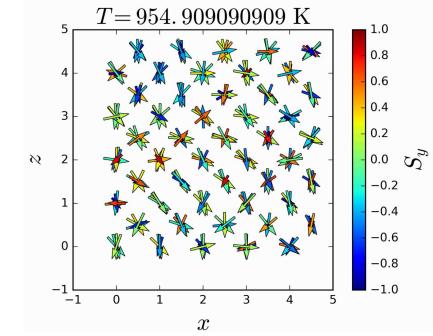
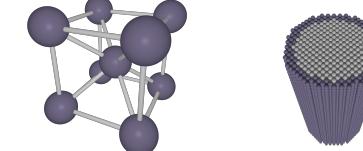
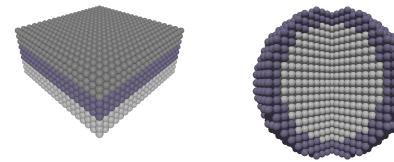
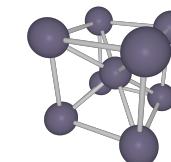
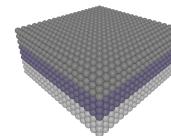
Construcción

Simulación

Análisis de  
Resultados



<https://pcm-ca.github.io/vegas/>

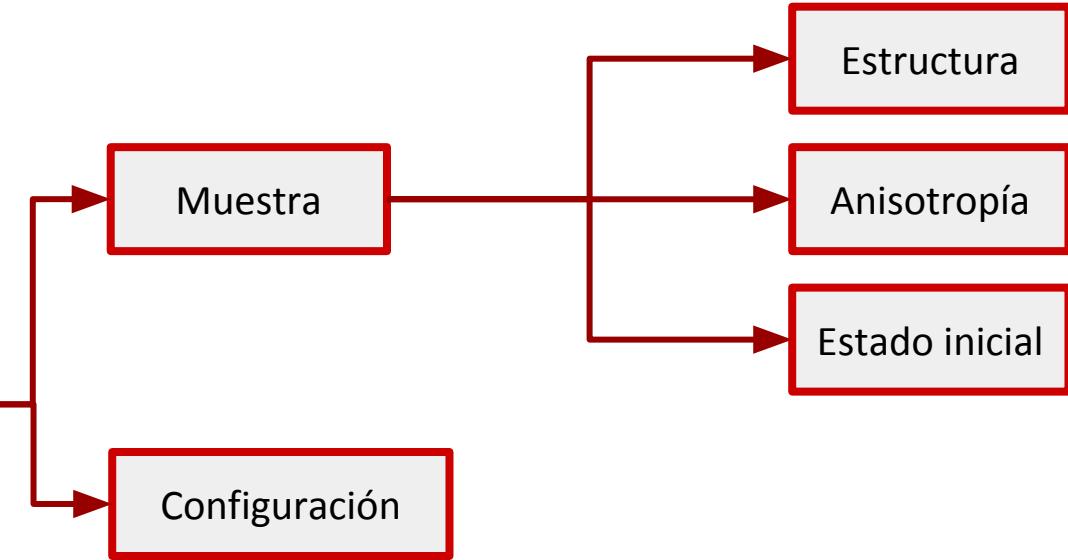


```
*****
** VEGAS
** PCM Computational Applications - 2017
** ****
A JSON file is necessary !!!
Unsuccessful completion !!!
```

Software



# Vegas



<https://pcm-ca.github.io/vegas/>

# Vegas (muestra)

num\_ions num\_interactions num\_types

type1

type2

...

index px py pz spin hx hy hz ion\_type update\_policy

...

index nbh\_index jex

0 100 1.0  
0 900 1.0  
0 10 1.0  
0 90 1.0  
0 1 1.0  
0 9 1.0  
1 101 1.0  
1 901 1.0  
1 11 1.0  
1 91 1.0  
1 2 1.0  
1 0 1.0  
2 102 1.0  
2 902 1.0  
2 12 1.0  
2 92 1.0  
2 3 1.0  
2 1 1.0  
3 103 1.0  
3 903 1.0

1000 6000 1  
generic  
0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
1 0.0 0.0 1.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
2 0.0 0.0 2.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
3 0.0 0.0 3.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
4 0.0 0.0 4.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
5 0.0 0.0 5.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
6 0.0 0.0 6.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
7 0.0 0.0 7.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
8 0.0 0.0 8.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
9 0.0 0.0 9.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
10 0.0 1.0 0.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
11 0.0 1.0 1.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
12 0.0 1.0 2.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
13 0.0 1.0 3.0 1.0 0.0 0.0 0.0 1.0 generic adaptive  
14 0.0 1.0 4.0 1.0 0.0 0.0 0.0 1.0 generic adaptive

# Vegas (configuración)

Json

```
{  
    "sample": "sample.dat",  
    "anisotropy": "anisotropy.dat",  
    "initialstate": "initialstate.dat",  
    "out": "results.h5",  
    "mcs": 10000,  
    "seed": 5681401,  
    "kb": 0.08618,  
    "field": 0.0,  
    "temperature": 100.0  
}
```



# Vegas (ejecución)



```
*****
**          VEGAS
**          PCM Computational Applications - 2017
**
*****
Sample file = sample.dat
Num MCS = 10000
Out file = results.h5
Anisotropy file = anisotropy.dat

Num Ions = 250
Num Fe Ions = 250
kb = 0.08618
seed = 5681401

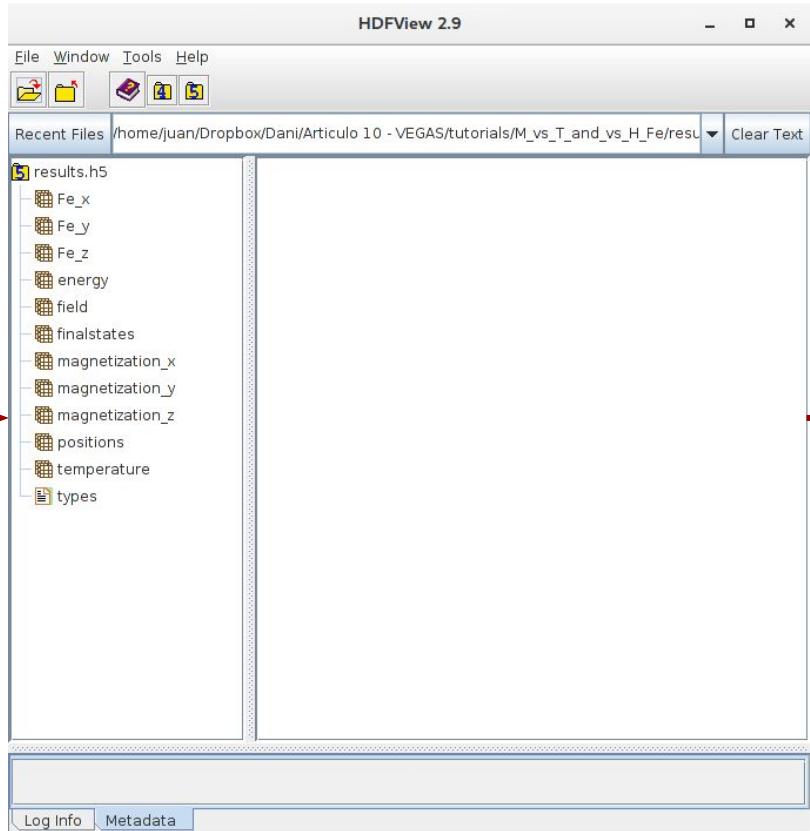
ETR: 0:1:40 (1.00000%) ==> T = 1500.00000; H = 0.00000 Fe 60.00000
ETR: 0:2:28 (2.00000%) ==> T = 1484.85859; H = 0.00000 Fe 60.00000
ETR: 0:2:10 (3.00000%) ==> T = 1469.71717; H = 0.00000 Fe 60.00000
ETR: 0:2:01 (4.00000%) ==> T = 1454.57576; H = 0.00000 Fe 60.00000
ETR: 0:1:55 (5.00000%) ==> T = 1439.43434; H = 0.00000 Fe 60.00000
ETR: 0:1:50 (6.00000%) ==> T = 1424.29293; H = 0.00000 Fe 60.00000
ETR: 0:1:47 (7.00000%) ==> T = 1409.15152; H = 0.00000 Fe 60.00000
ETR: 0:1:44 (8.00000%) ==> T = 1394.01010; H = 0.00000 Fe 60.00000
ETR: 0:1:52 (9.00000%) ==> T = 1378.86869; H = 0.00000 Fe 60.00000
ETR: 0:1:49 (10.00000%) ==> T = 1363.72727; H = 0.00000 Fe 60.00000
ETR: 0:1:46 (11.00000%) ==> T = 1348.58586; H = 0.00000 Fe 60.00000
ETR: 0:1:43 (12.00000%) ==> T = 1333.44444; H = 0.00000 Fe 60.00000
ETR: 0:1:41 (13.00000%) ==> T = 1318.30303; H = 0.00000 Fe 60.00000
ETR: 0:1:39 (14.00000%) ==> T = 1303.16162; H = 0.00000 Fe 60.00000
ETR: 0:1:43 (15.00000%) ==> T = 1288.02020; H = 0.00000 Fe 60.00000
```

# Vegas (ejecución)

```
*****
**          VEGAS
**          ****
**          PCM Computational Applications - 2017
**          ****
Sample file =
    sample.dat
Num MCS =
    10000
Out file =
    results.h5
Anisotropy file =
    anisotropy.dat

Num Ions =
    250
Num Fe Ions =
    250
kb =
    0.08618
seed =
    5681401

ETR: 0:1:40   (1.00000%) ==> T = 1500.00000; H = 0.00000 Fe 60.00000
ETR: 0:2:28   (2.00000%) ==> T = 1484.85859; H = 0.00000 Fe 60.00000
ETR: 0:2:10   (3.00000%) ==> T = 1469.71717; H = 0.00000 Fe 60.00000
ETR: 0:2:01   (4.00000%) ==> T = 1454.57576; H = 0.00000 Fe 60.00000
ETR: 0:1:55   (5.00000%) ==> T = 1439.43434; H = 0.00000 Fe 60.00000
ETR: 0:1:50   (6.00000%) ==> T = 1424.29293; H = 0.00000 Fe 60.00000
ETR: 0:1:47   (7.00000%) ==> T = 1409.15152; H = 0.00000 Fe 60.00000
ETR: 0:1:44   (8.00000%) ==> T = 1394.01010; H = 0.00000 Fe 60.00000
ETR: 0:1:52   (9.00000%) ==> T = 1378.86869; H = 0.00000 Fe 60.00000
ETR: 0:1:49   (10.00000%) ==> T = 1363.72727; H = 0.00000 Fe 60.00000
ETR: 0:1:46   (11.00000%) ==> T = 1348.58586; H = 0.00000 Fe 60.00000
ETR: 0:1:43   (12.00000%) ==> T = 1333.44444; H = 0.00000 Fe 60.00000
ETR: 0:1:41   (13.00000%) ==> T = 1318.30303; H = 0.00000 Fe 60.00000
ETR: 0:1:39   (14.00000%) ==> T = 1303.16162; H = 0.00000 Fe 60.00000
ETR: 0:1:43   (15.00000%) ==> T = 1288.02020; H = 0.00000 Fe 60.00000
```



# Vegas (resultados)

