1st International Applied Physics Engineering & Innovation

6th National Conference of Physical Engineering

PCM Computational Applications

UNIVERSIDAD NACIONAL DE COLOMBIA

Simulación de sistemas magnéticos por medio del método Monte Carlo

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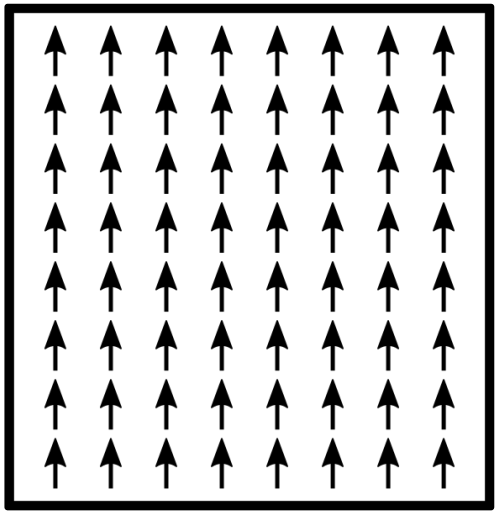
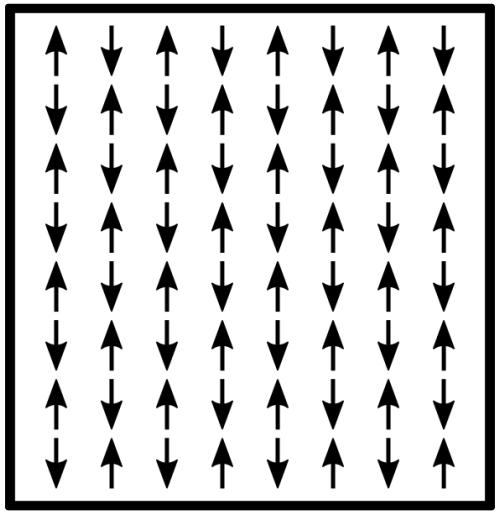
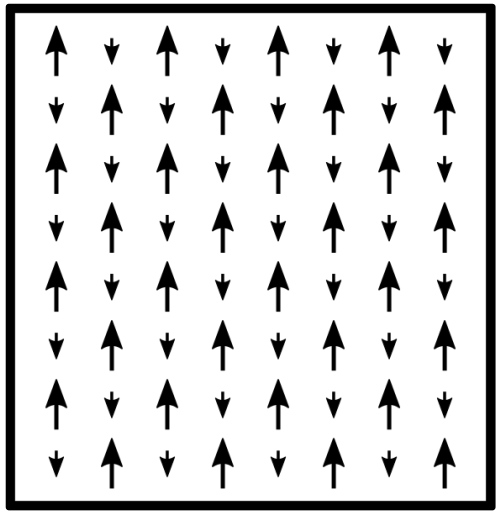
Fundamentación teórica



Ferromagnético
(FM)

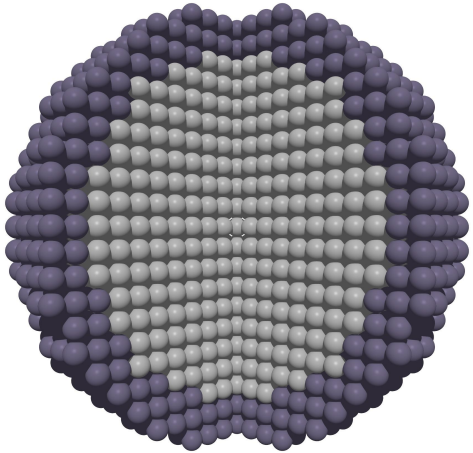


Antiferromagnético
(AFM)

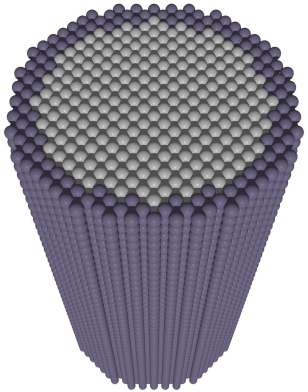


Ferrimagnético
(FiM)

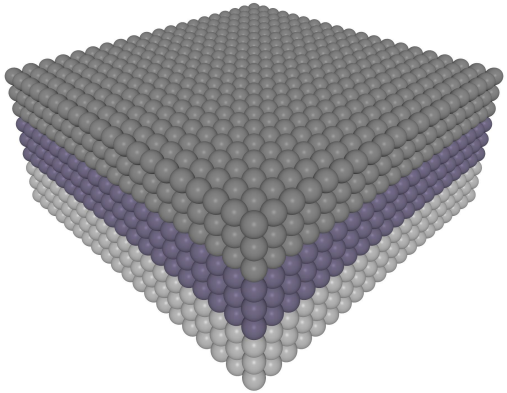
Nanoestructuras magnéticas



Nanopartícula
core/shell



Nanohilo
core/shell

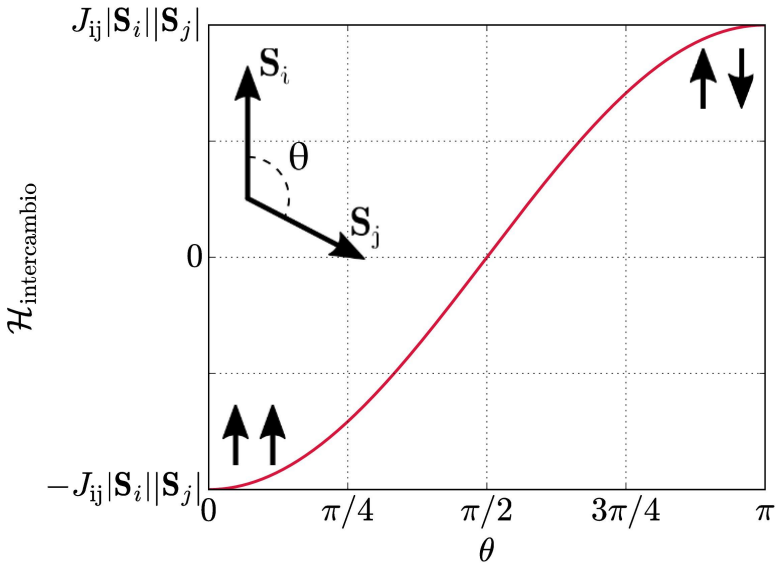


Multicapas

Términos energéticos

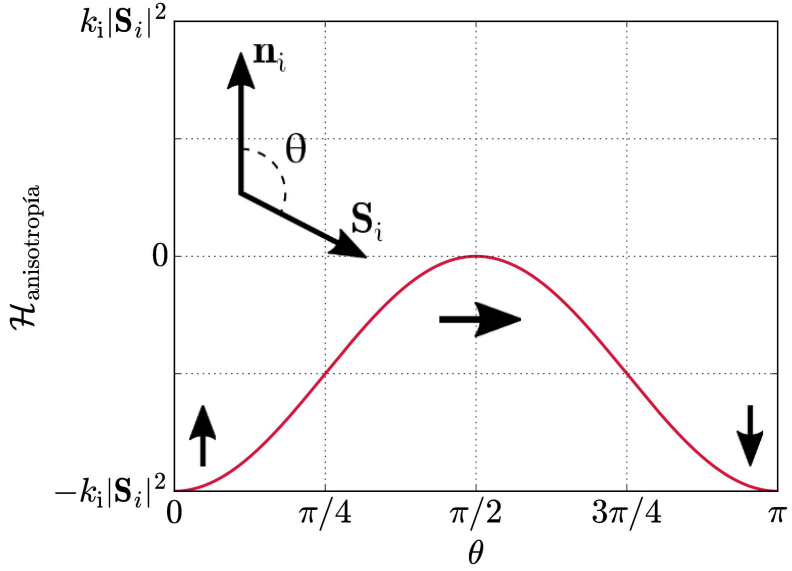
Intercambio magnético

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



Anisotropía magnetocristalina

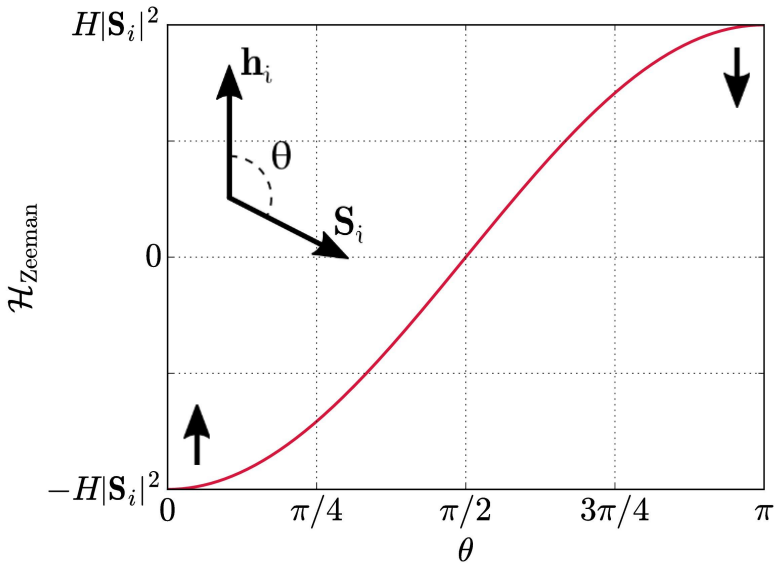
$$\mathcal{H}_{\text{anisotropia}} = -\sum_{i} k_i \left(\boldsymbol{S}_i \cdot \boldsymbol{n}_i\right)^2$$

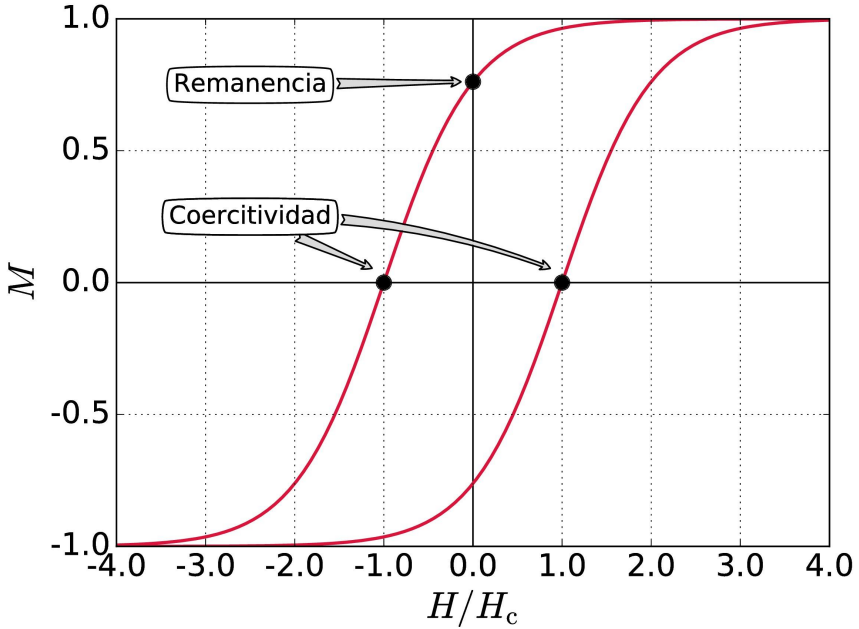


Términos energéticos

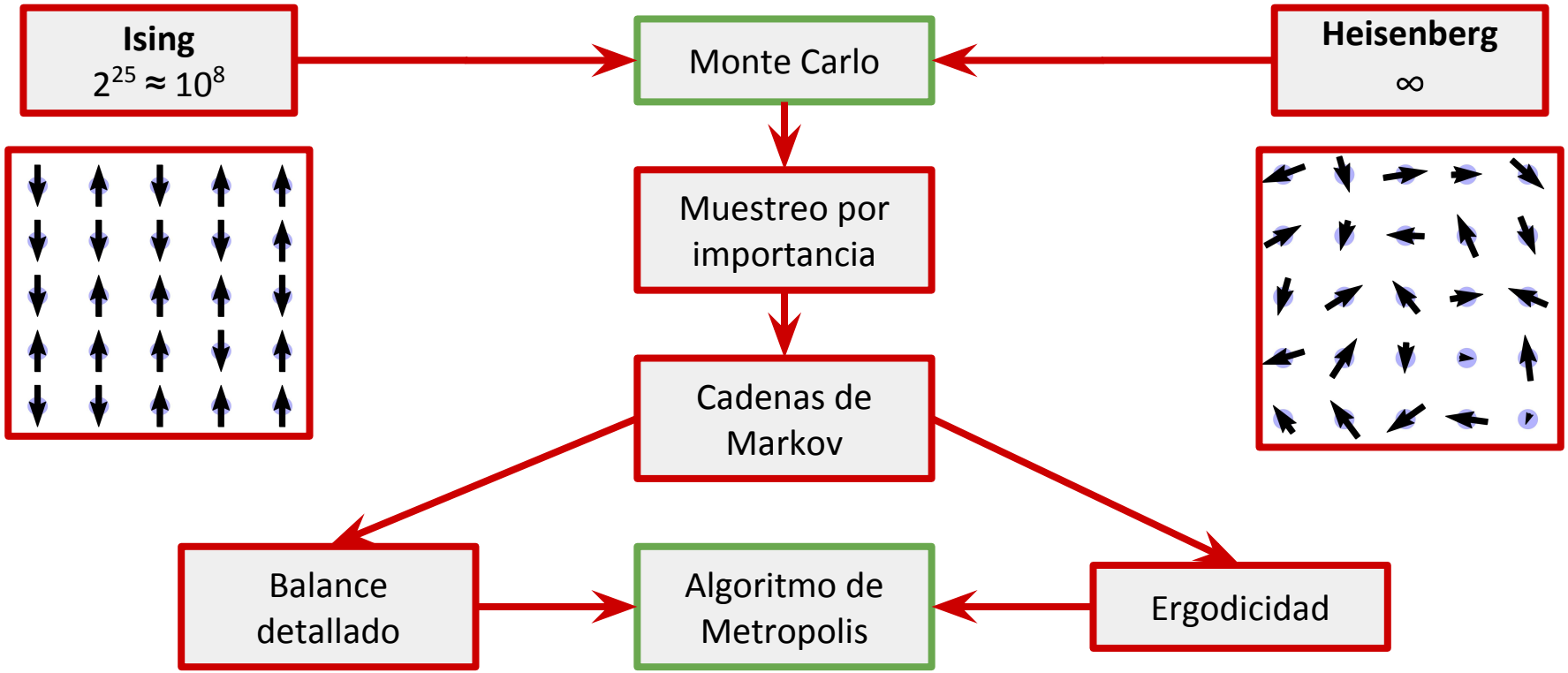
Influencia de un campo externo

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

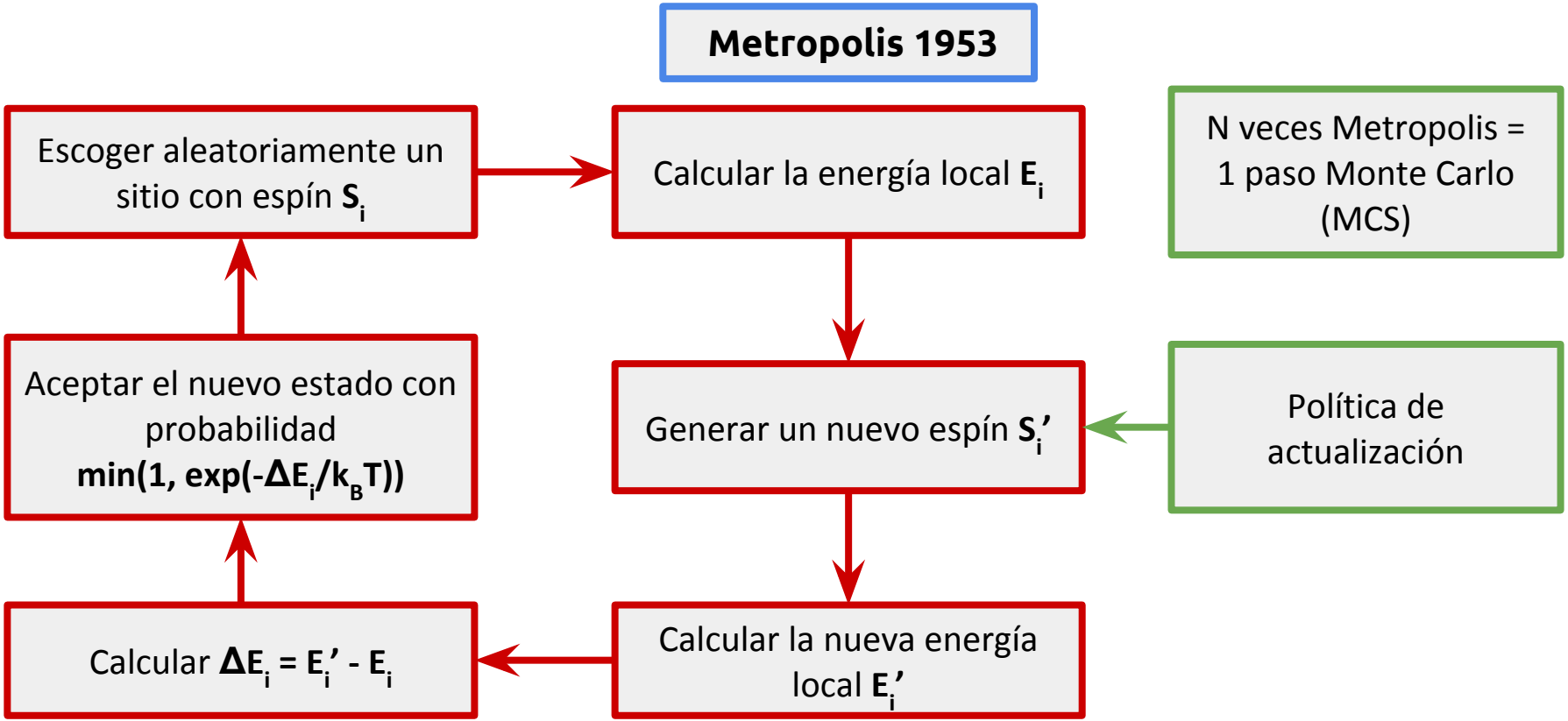




Método Monte Carlo

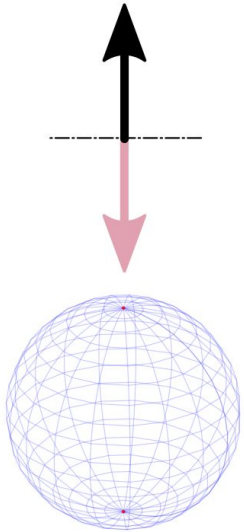


Algoritmo de Metropolis



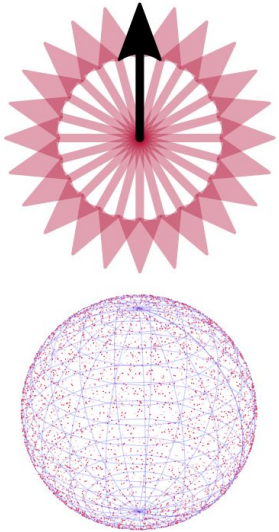
Políticas de actualización

Spin flip



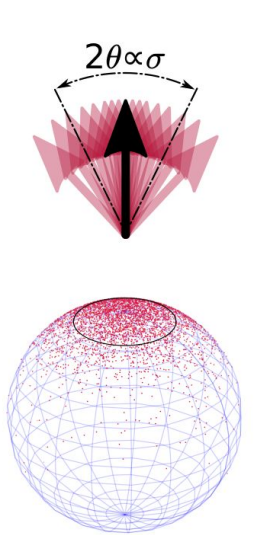
$$S'_i = -S_i$$

Aleatoria



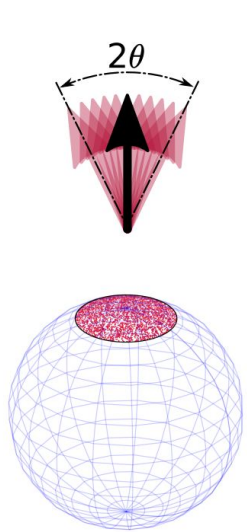
$$S'_i = \frac{\Gamma}{|\Gamma|}$$

Gaussiana



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

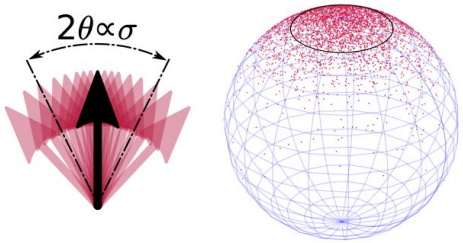
Small step



Algoritmo Adaptativo

Gaussiana

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



Tasa de aceptación:
R = R(σ, ΔE, T)

σ

σ → 0 → **R** alta → Muestreo lento del espacio de fases.

σ → ∞ → **R** baja → Rechazamiento de casi todos los nuevos estados.

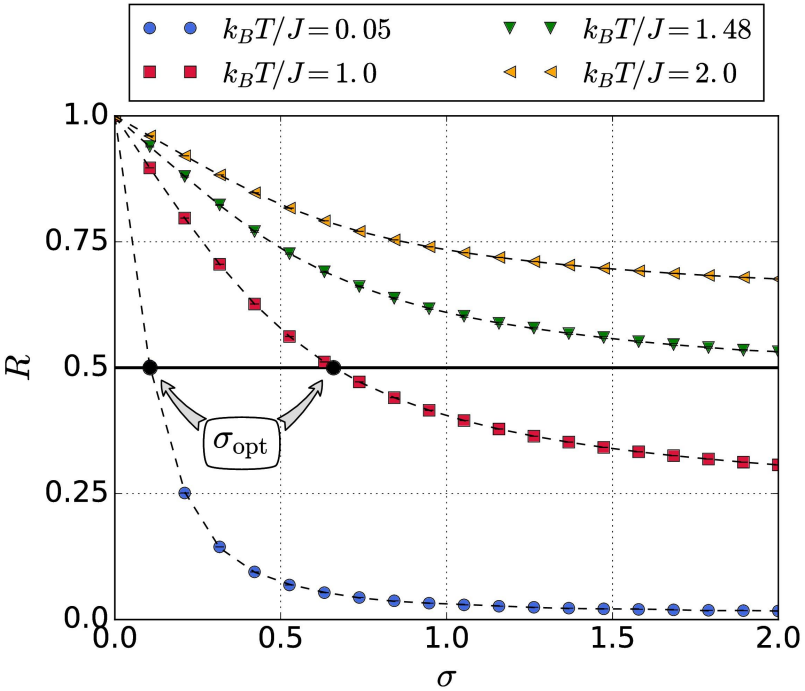
R ≈ 0.5

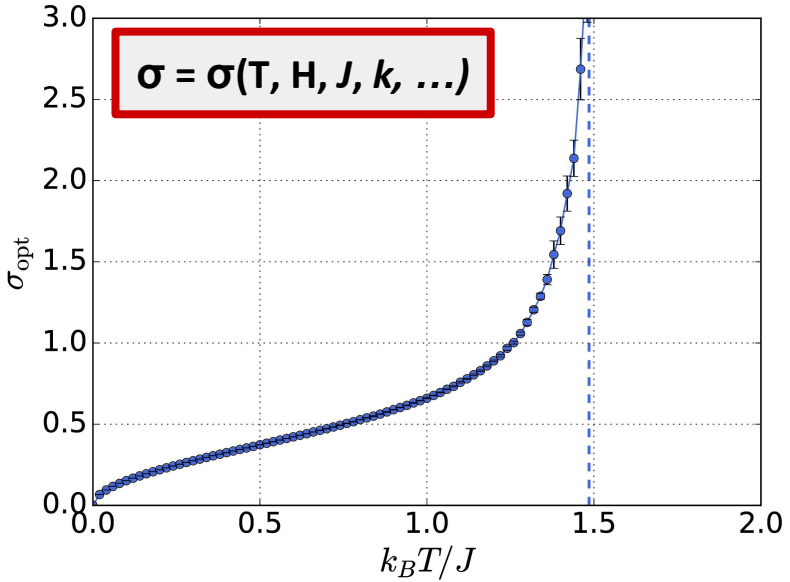
Algoritmo Adaptativo

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

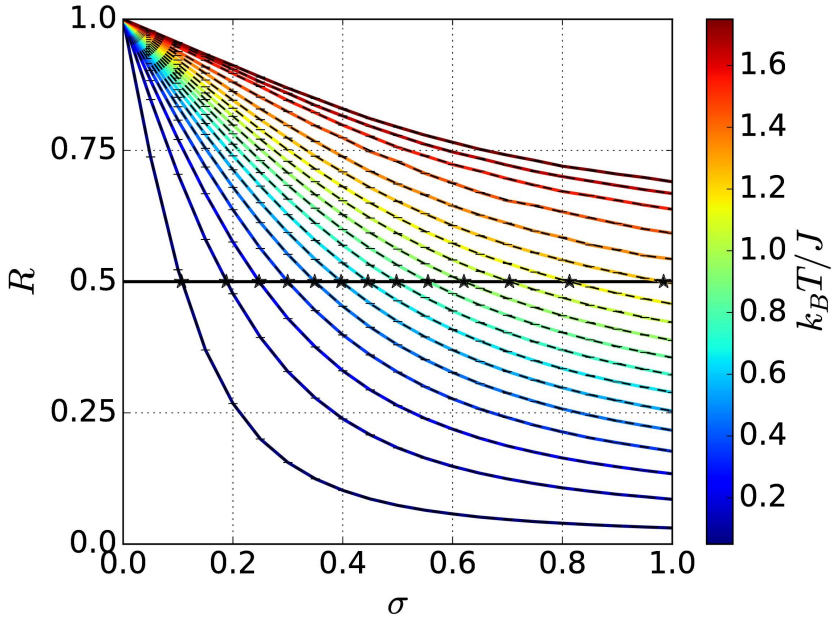
$$\begin{aligned} J &= 1.0 \\ k &= 0.001J \end{aligned}$$

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

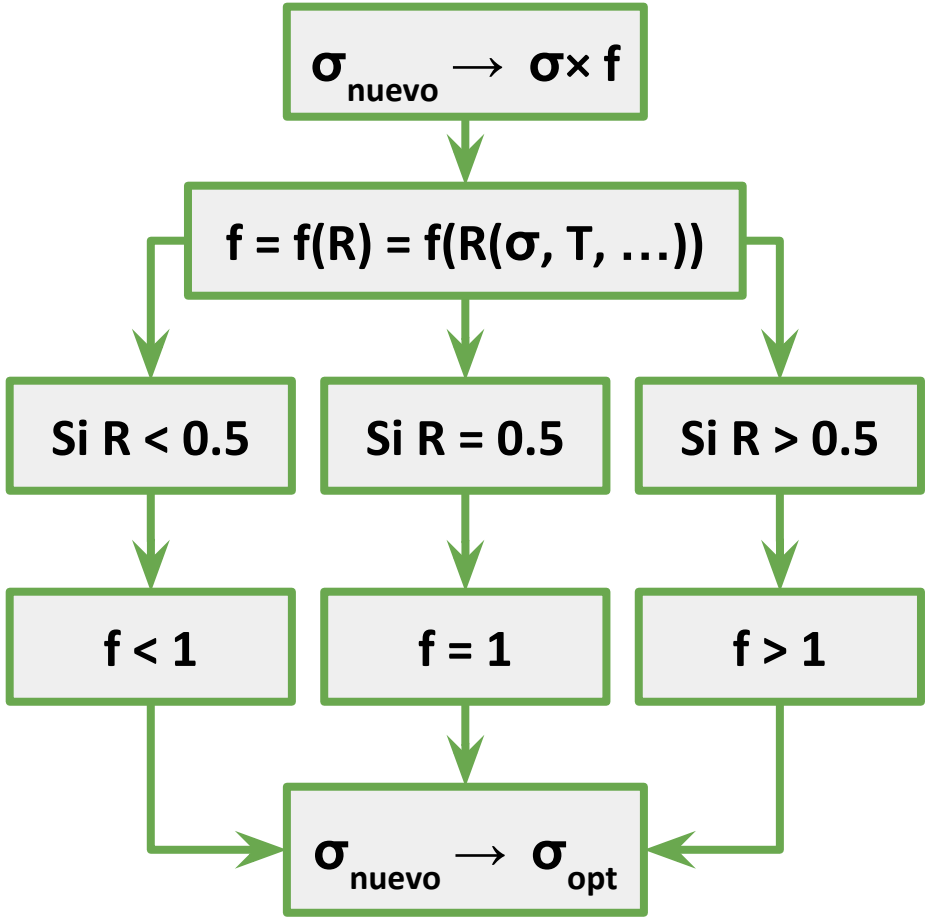




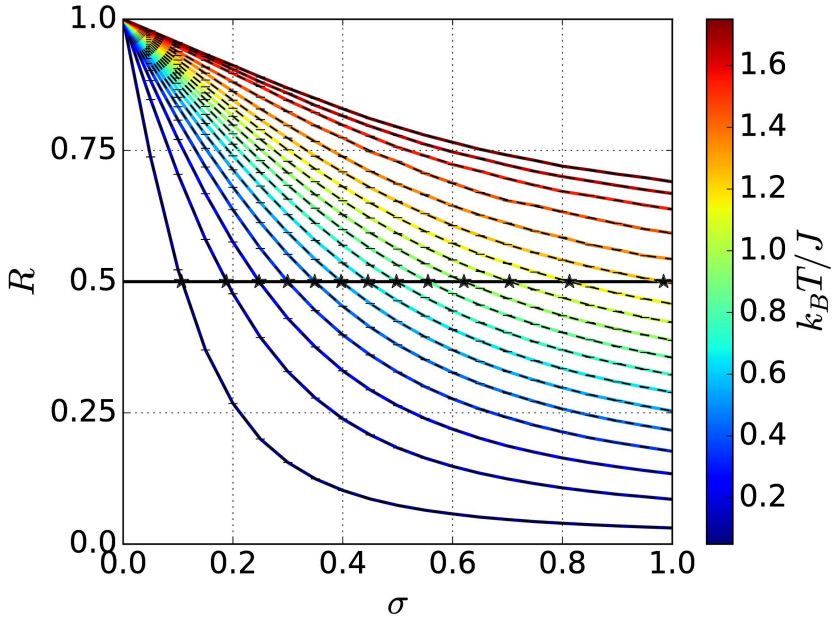
Algoritmo Adaptativo



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

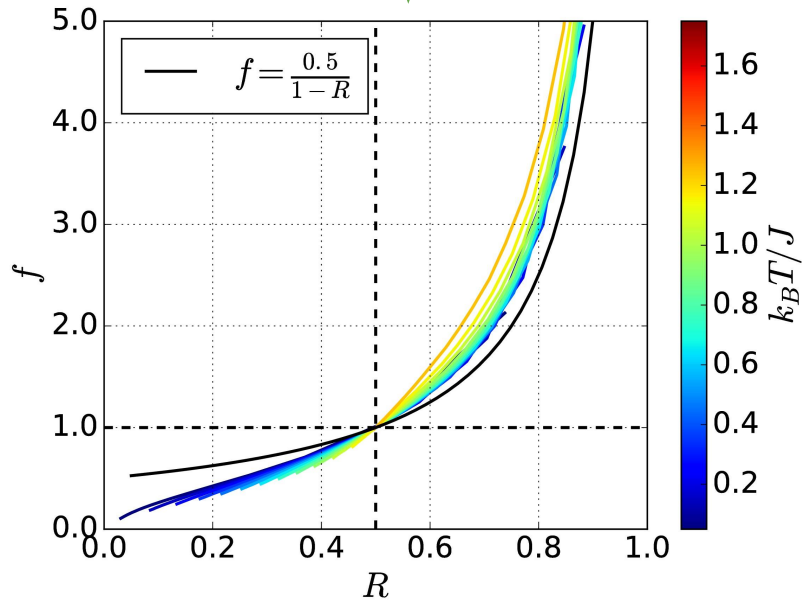


Algoritmo Adaptativo

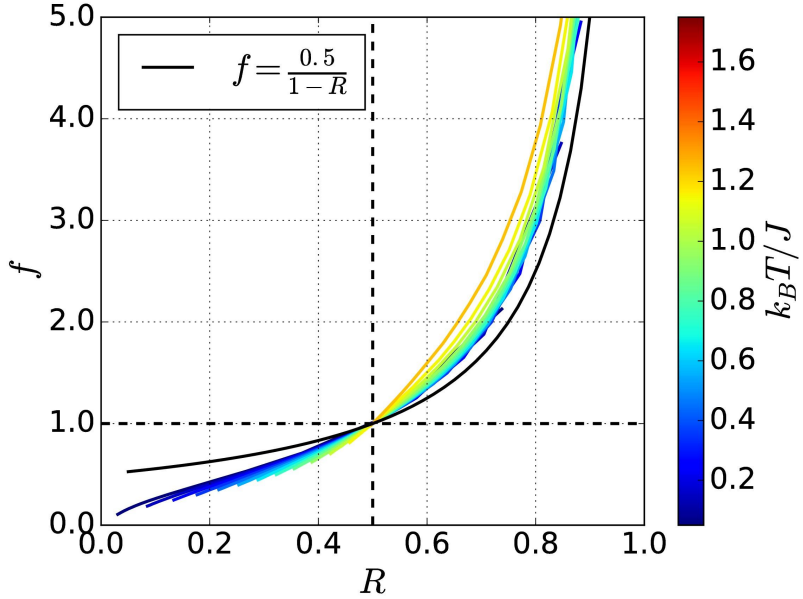


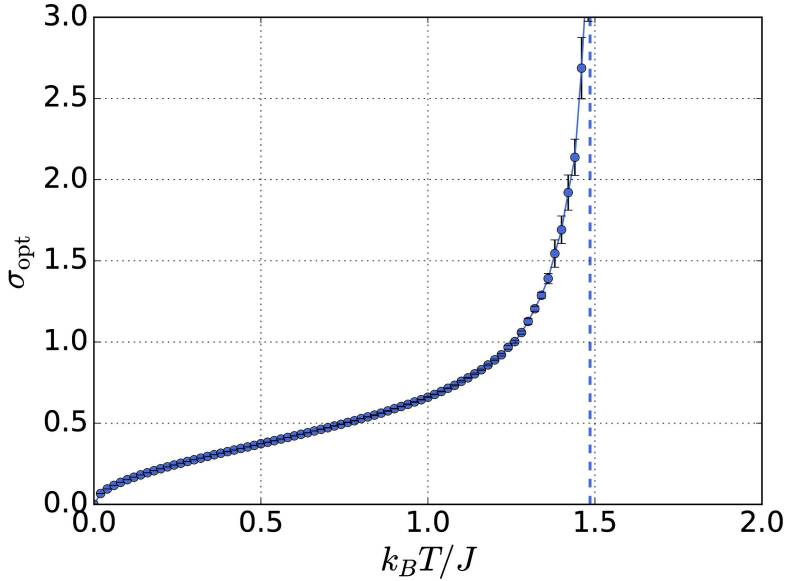
$$\frac{k_B T_C}{J} = 1.485427$$

f = σ$_{opt}$ / σ



Algoritmo Adaptativo





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

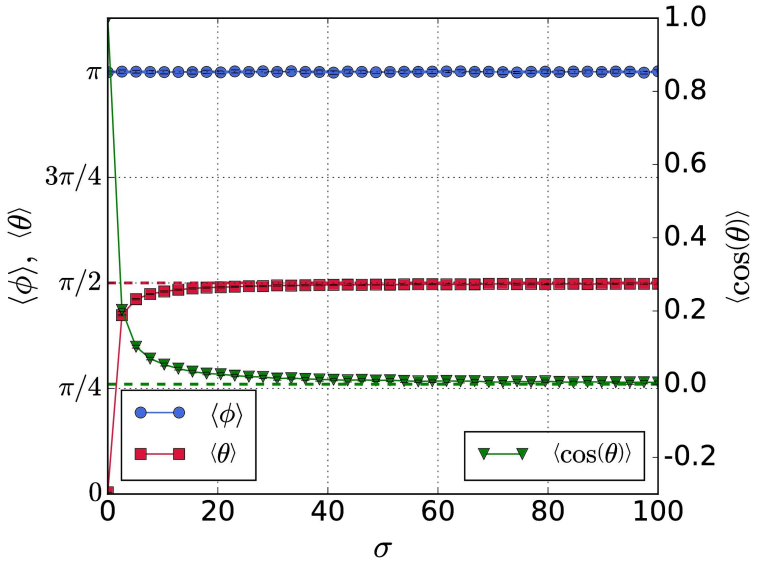
Si **T ≥ T$_c$** → **R > 0.5** → **f > 1** → **σ** diverge

Algoritmo Adaptativo

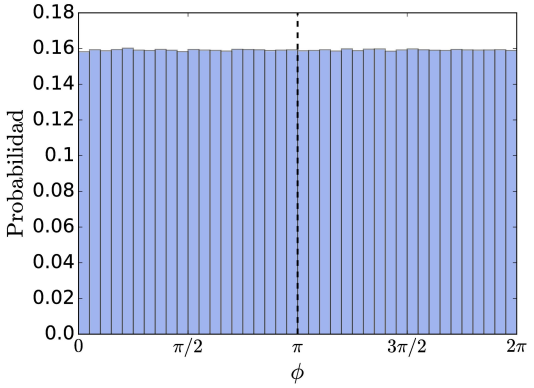
Gaussiana

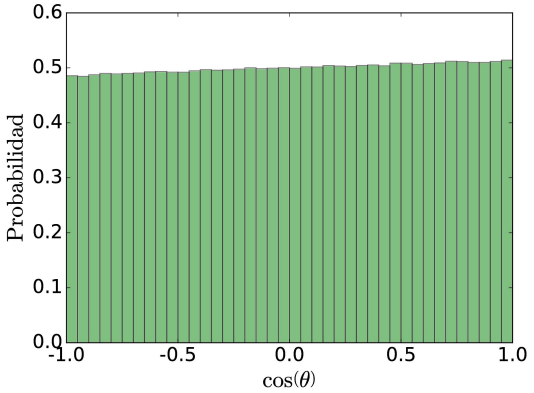
Aleatoria

$$S_i' = \frac{S_i + \sigma\Gamma}{|S_i + \sigma\Gamma|} \xrightarrow{\sigma \to \infty} S_i' = \frac{\Gamma}{|\Gamma|}$$

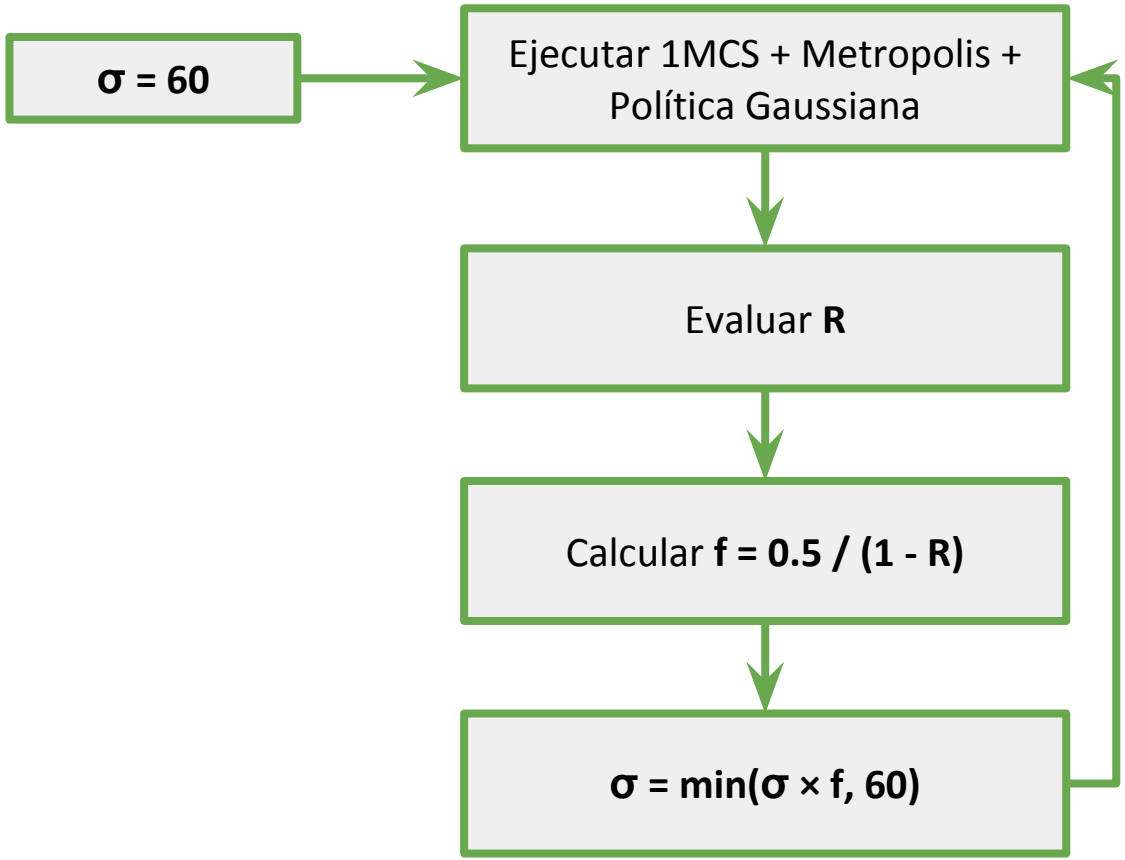


$\sigma_{máx} = 60$





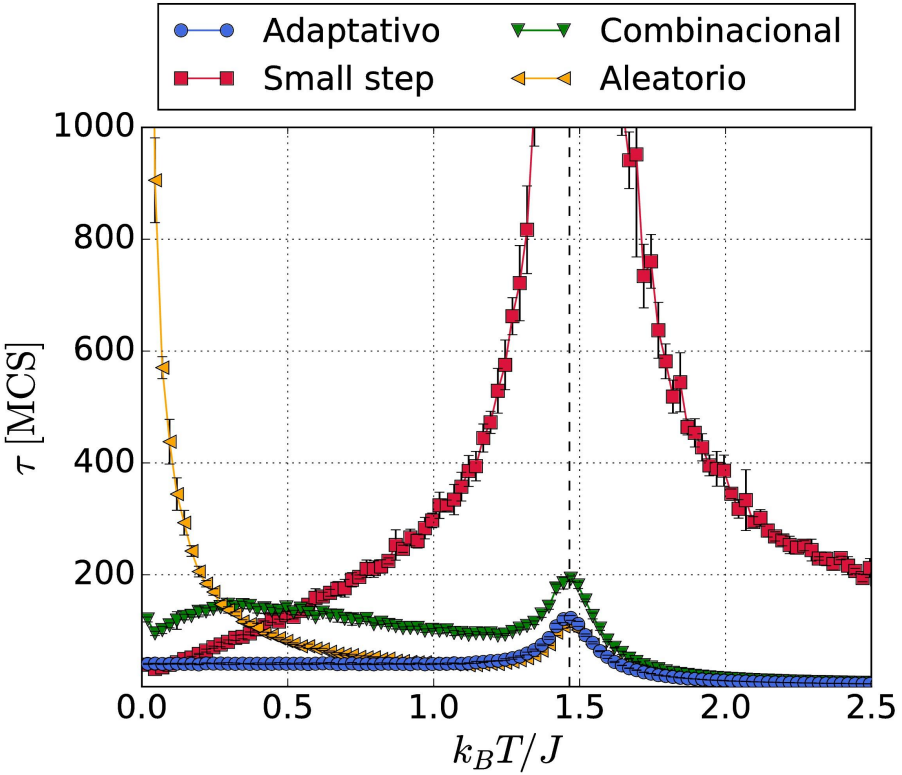
Algoritmo Adaptativo



Regla de oro
R ≈ 0.5

Algoritmo Adaptativo

Tiempos de correlación



Adaptativo es hasta 20 veces mejor que Aleatorio

Vegas

Algoritmo Adaptativo

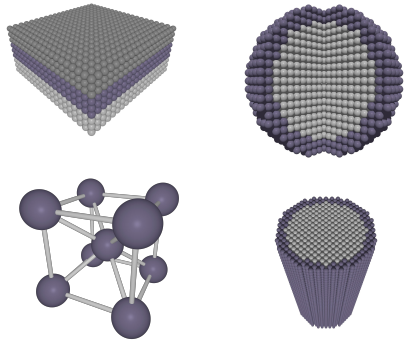
https://pcm-ca.github.io/vegas/

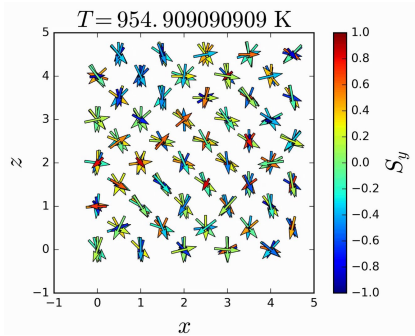
GitHub

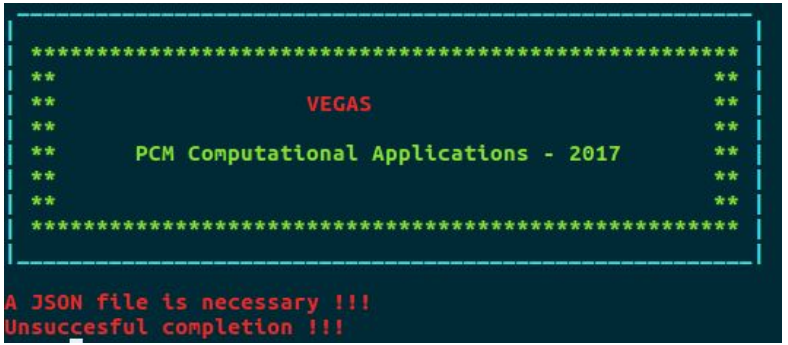
Construcción

Simulación

Análisis de Resultados



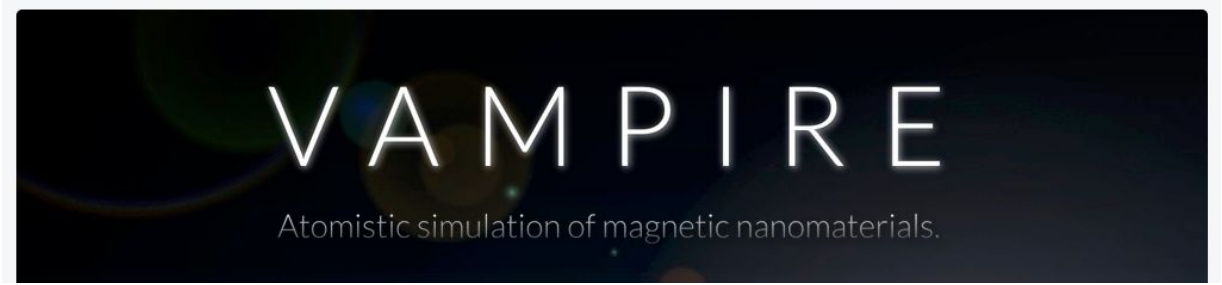




Software

Spin

juDFT



¿

Fácil
Versátil
Unificado
Propio

?

Vegas

- Muestra
  - Estructura
  - Anisotropía
  - Estado inicial
- Configuración

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

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

```
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
```

Vegas (configuración)

Json

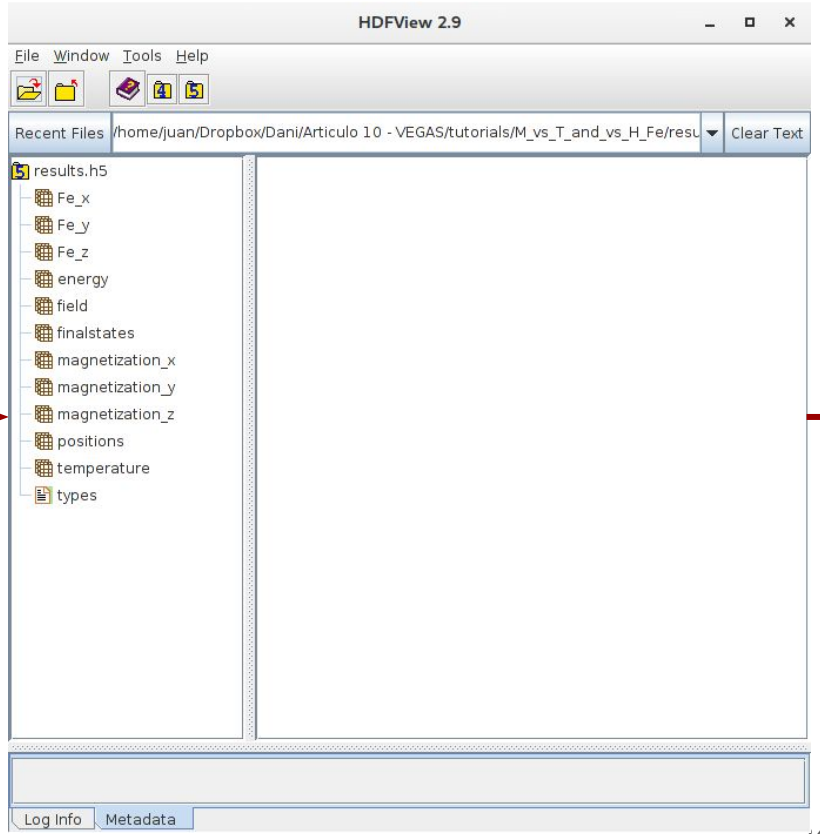
```
{
    "sample": "sample.dat",
    "anisotropy": "anisotropy.dat",
    "initialstate": "initialstate.dat",
    "out": "results.h5",
    "mcs": 10000,
    "seed": 5681401,
    "kb": 0.08618,
    "field": 0.0,
    "temperature": 100.0
}
```

Vegas (ejecución)

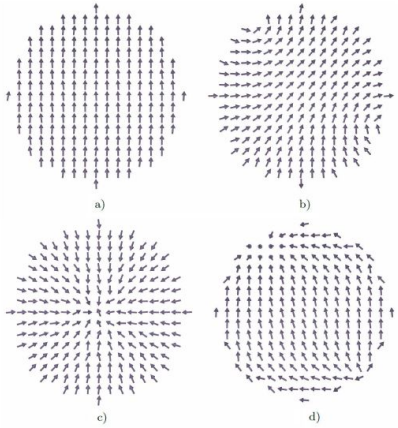

```
**************************************************
**                                              **
**                  VEGAS                       **
**                                              **
**      PCM Computational Applications - 2017   **
**                                              **
**                                              **
**************************************************

              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
```

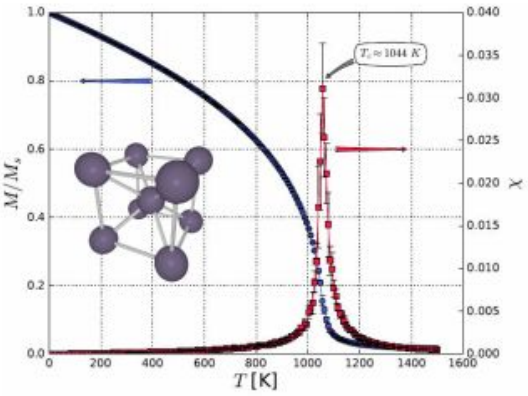
Vegas (ejecución)

```
**************************************************
**                                              **
**                  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
```

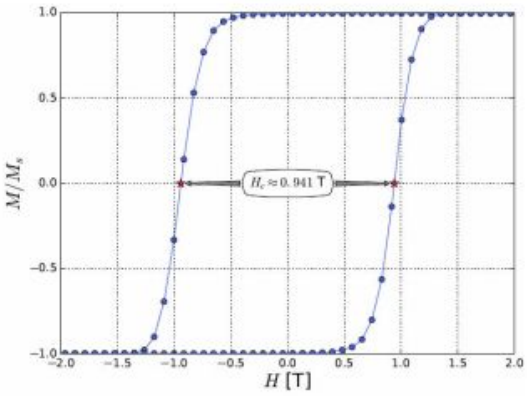


Vegas (resultados)





a)



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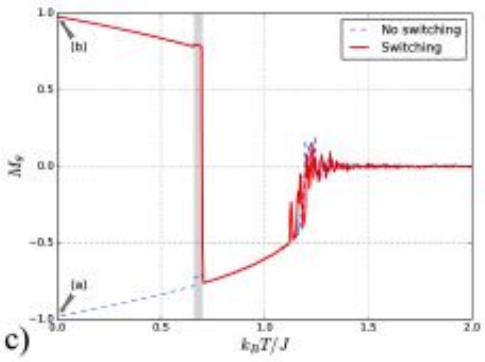

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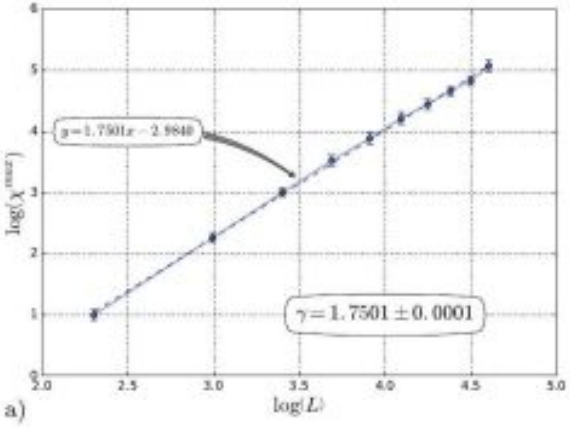

a)