



Modelli di spin

Simulazione di Materia Condensata e Biosistemi

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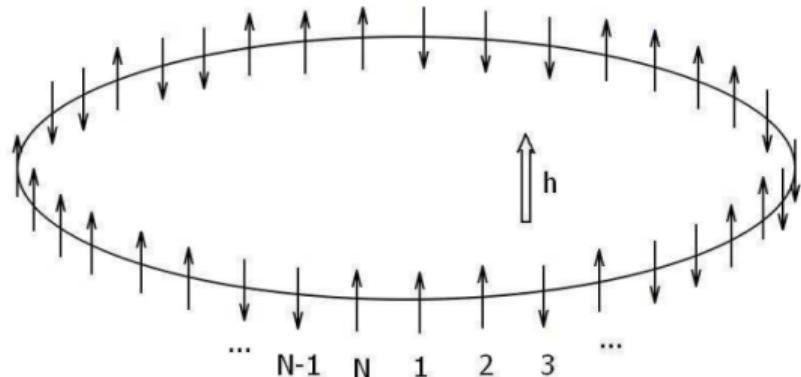


Hamiltoniana

1 Introduzione

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i$$

- ◊ Interazione fra primi vicini
- ◊ Accoppiamento con un campo esterno



Modello di Ising 1D con condizioni periodiche.



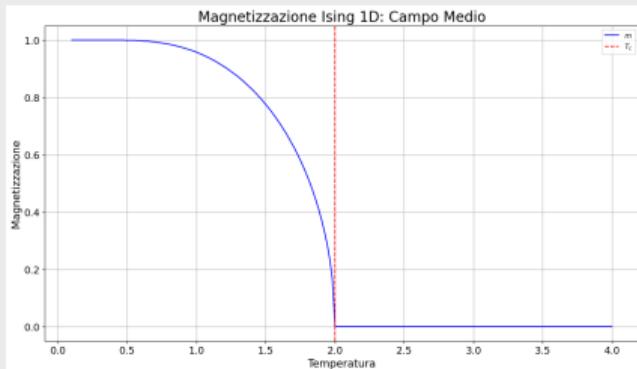
Modello di Ising 1D

1 Introduzione

Campo medio

- ◊ Transizione di fase a $T_c \neq 0$

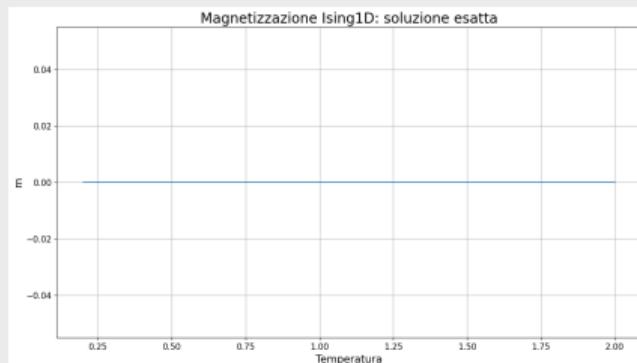
$$m = \tanh [\beta (h + Jn_{nn}m)]$$



Soluzione analitica

- ◊ No magnetizzazione se $T \neq 0, h = 0$

$$m = \frac{\sinh(\beta h)}{\sqrt{e^{-4\beta J} + \sinh^2(\beta h)}}$$



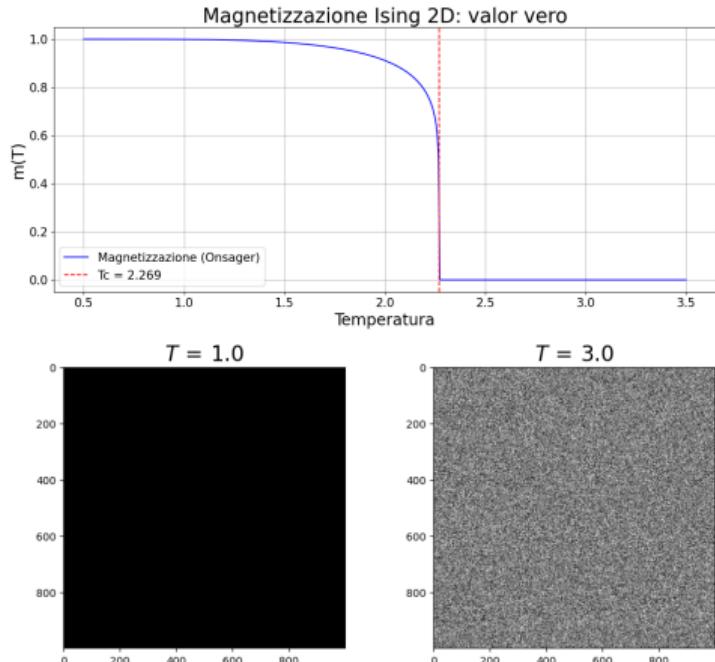


Modello di Ising 2D

1 Introduzione

- ◊ Soluzione analitica per $h = 0$
- ◊ Sistema presenta una transizione di fase a $T_c \neq 0$

$$m(\beta, h=0) = \begin{cases} \left[1 - \frac{1}{\sinh^4(2\beta J)}\right]^{\frac{1}{8}} & T < T_c \\ 0 & T > T_c \end{cases}$$





Modello XY

1 Introduzione

Hamiltoniana

$$H = -J \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j - \sum_i \vec{h} \cdot \vec{s}_i$$

- ◊ Simmetria continua
- ◊ Difetti topologici (vortici)

Modello XY

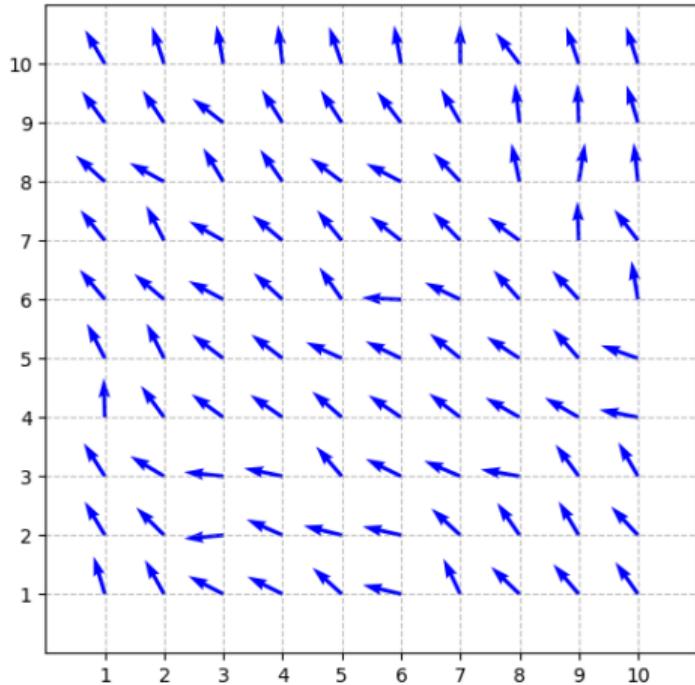




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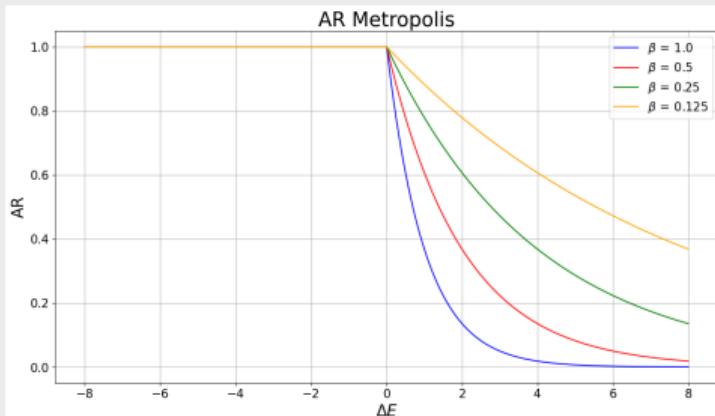


Metropolis vs Wolff

2 Metodi numerici

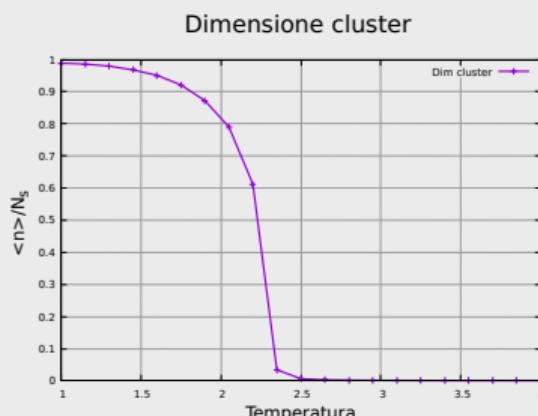
Metropolis

- ◊ Tentata inversione di un singolo spin
- ◊ $A(\nu | \mu) = \min [1, e^{-\beta(E_\nu - E_\mu)}]$
- ◊ Ottimo per $T \ll T_c$ oppure $T \gg T_c$



Wolff

- ◊ Algoritmo di clustering
- ◊ $P_{add} = 1 - \exp(-2\beta J)$
- ◊ Ottimo per $T \simeq T_c$

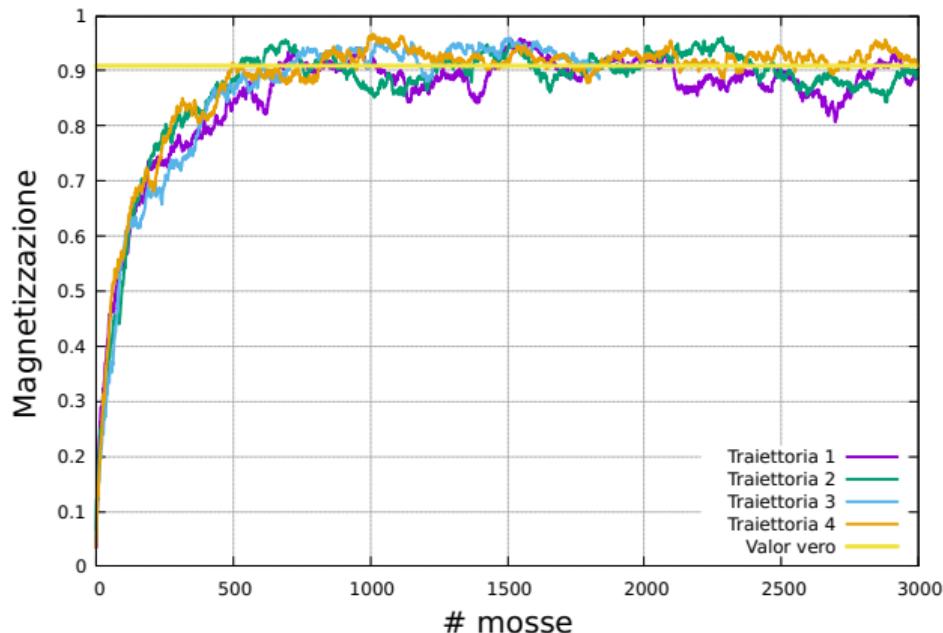




Termalizzazione

2 Metodi numerici

Termalizzazione: 6000 spin, $T = 0.5$



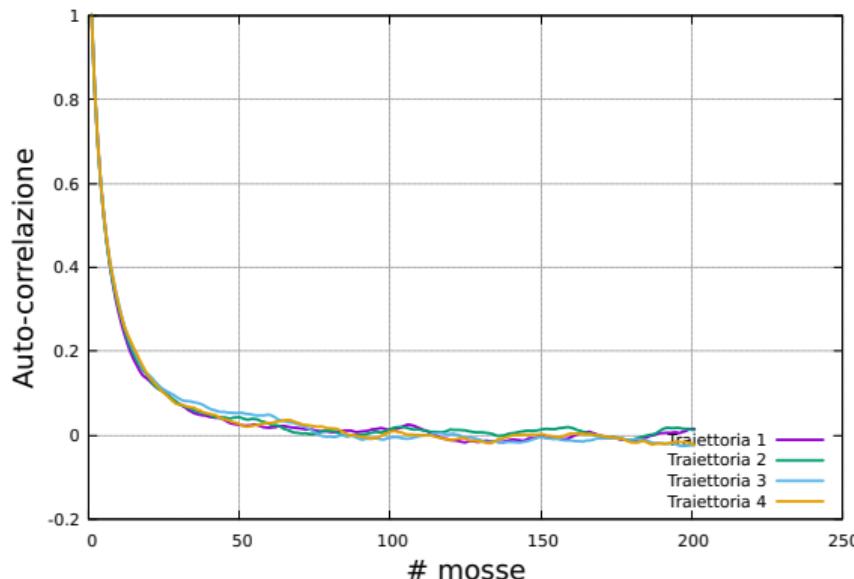
- ◊ Giungere all'equilibrio termodinamico
- ◊ Attenzione a stati metastabili
- ◊ Dipendenza dalla condizione iniziale



Auto-correlazione

2 Metodi numerici

Autocorrelazione m: N = 500, T = 2.0



Autocorrelazione per modello di Ising 2D.

Definizione

$$\chi(t) = \frac{\langle m(t')m(t'+t) \rangle_{t'} - \langle m \rangle^2}{\sigma_m^2}$$

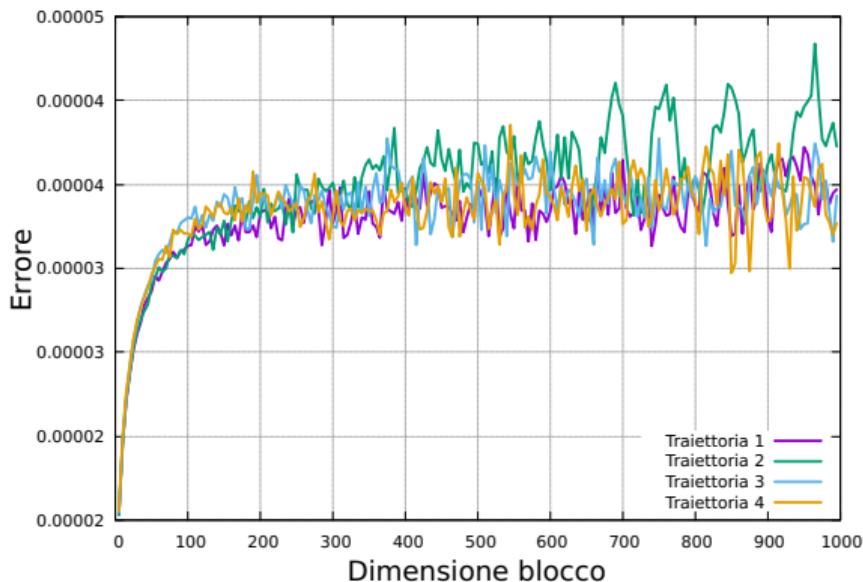
- ◊ $\chi(t) \propto e^{-t/t_c}$
- ◊ Indipendenza statistica fra configurazioni
- ◊ $n_{max} = \frac{t_{max}}{2t_c}$



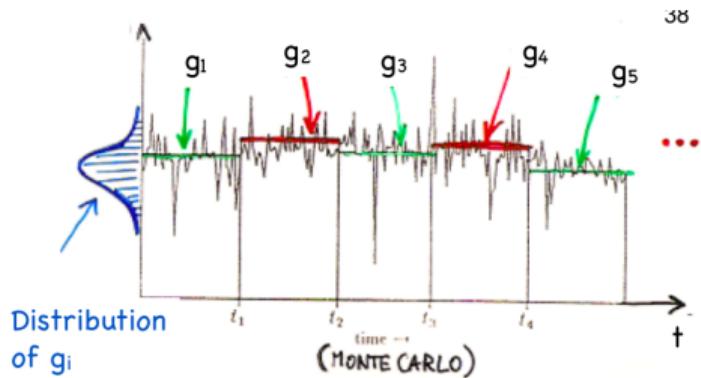
Data-blocking

2 Metodi numerici

Dimensione blocco: $N = 500$, $T = 2.0$



Analisi per dimensione blocchi nel caso di un modello di Ising 2D.



- ◊ Dati raggruppati in blocchi
- ◊ Errore satura quando raggiunta l_{lim}



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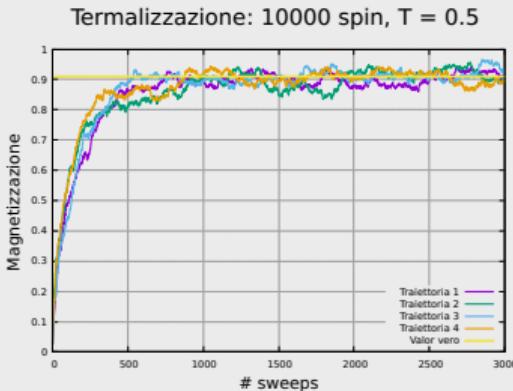


Caratterizzazione

3 Simulazioni modello di Ising 1D

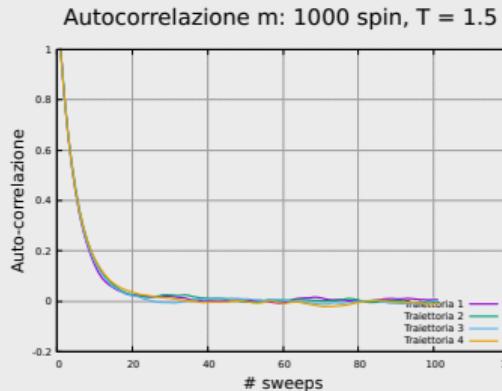
Termalizzazione

- ◊ Maggiore T, minore t_{ter}
- ◊ $t_{ter}^{max} \simeq 600$ sweeps



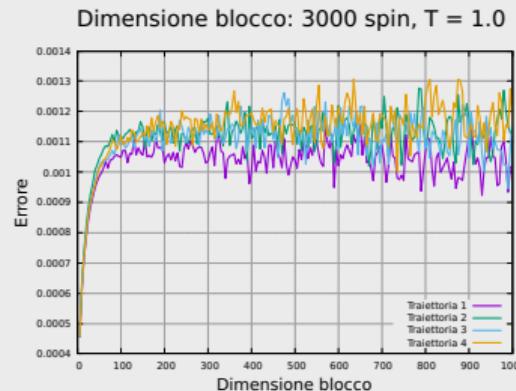
Auto-correlazione

- ◊ Maggiore T, minore t_c
- ◊ $t_c^{max} \simeq 500$ sweeps



Blocchi

- ◊ Maggiore T, minore l_{blk}
- ◊ $l_{blk}^{max} \simeq 1000$ sweeps

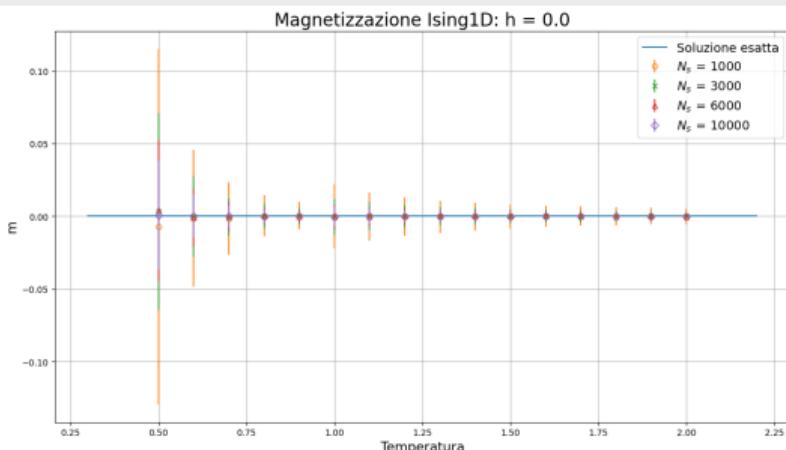




Magnetizzazione

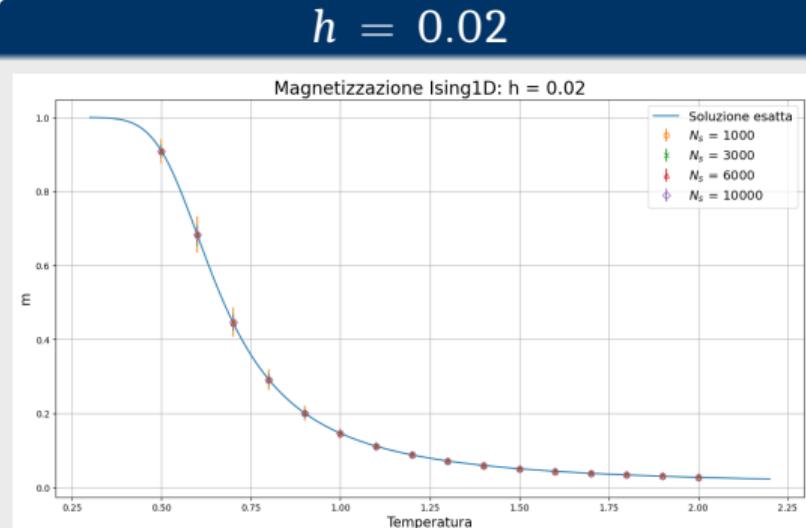
3 Simulazioni modello di Ising 1D

$$h = 0.0$$



◊ $m = 0$ per ogni $T \neq 0$

$$h = 0.02$$



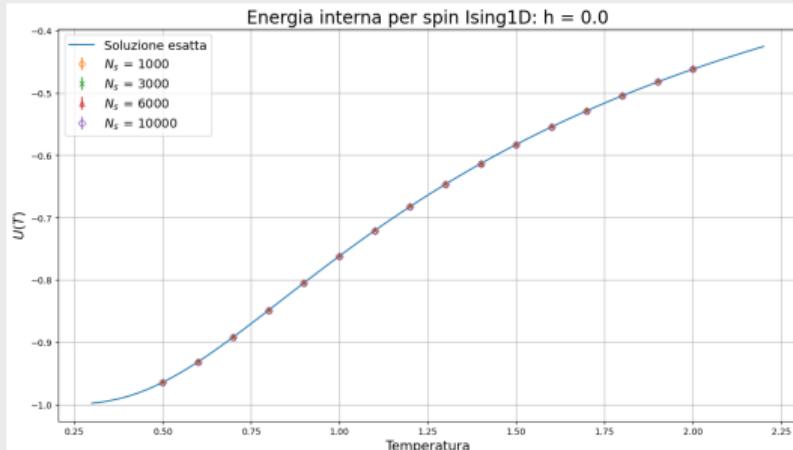
◊ campo magnetico impone ordine



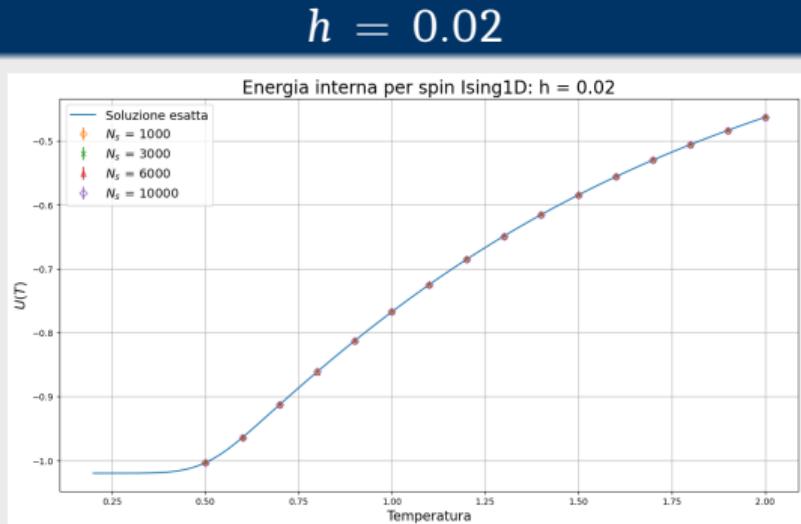
Energia interna

3 Simulazioni modello di Ising 1D

$$h = 0.0$$



$$h = 0.02$$



◊ per $T \rightarrow 0$ l'energia $U(T) \rightarrow -1$

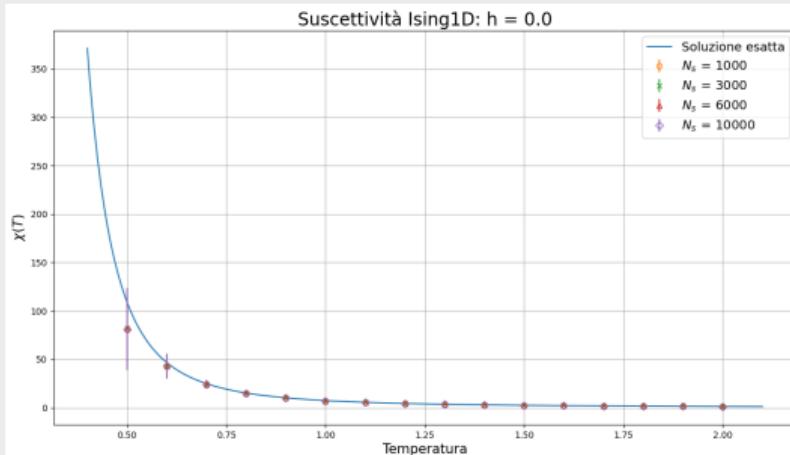
◊ per $T \rightarrow 0$ l'energia $U(T) \rightarrow -1.02$



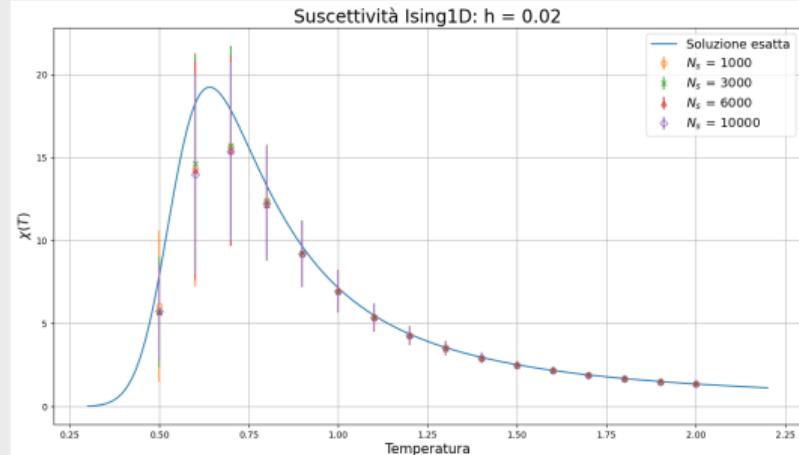
Suscettività magnetica

3 Simulazioni modello di Ising 1D

$h = 0.0$



$h = 0.02$



◊ aumento per $T \rightarrow 0$ perchè $T_c = 0$

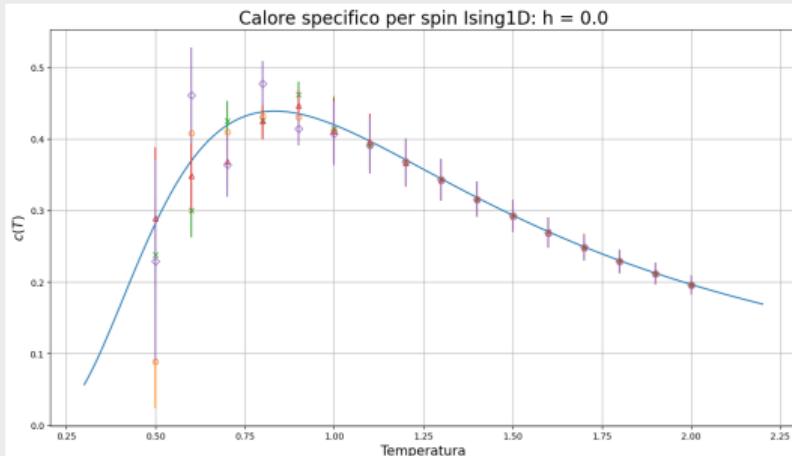
◊ picco a $T \neq 0$ dovuto ad h



Calore specifico

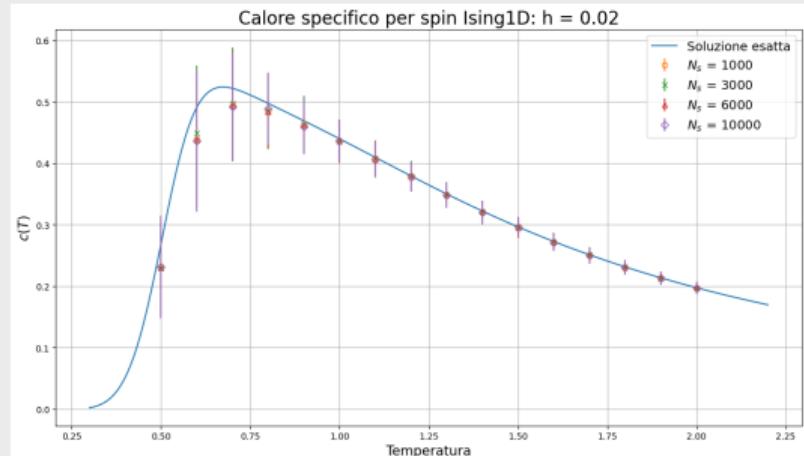
3 Simulazioni modello di Ising 1D

$h = 0.0$



◊ difficoltà a studiare il picco

$h = 0.02$



◊ campo magnetico semplifica lo studio



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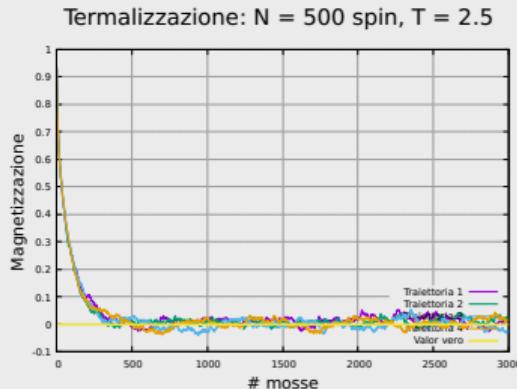


Caratterizzazione con metropolis

4 Simulazioni modello di Ising 2D

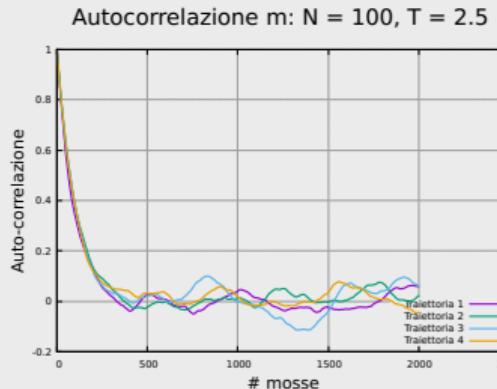
Termalizzazione

- ◊ t_{ter} maggiori per $T \simeq T_c$
- ◊ $t_{ter}^{max} \simeq 500$ sweeps



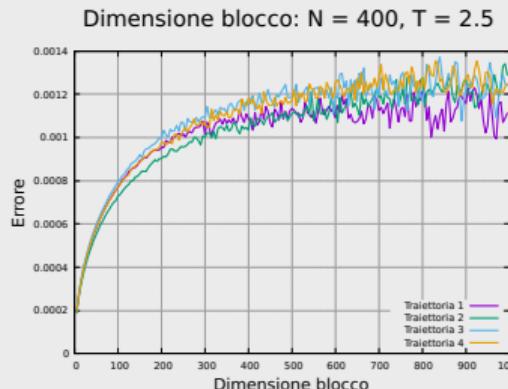
Auto-correlazione

- ◊ t_c maggiori per $T \simeq T_c$
- ◊ $t_c^{max} \simeq 400$ sweeps



Blocchi

- ◊ l_{blk} maggiori per $T \simeq T_c$
- ◊ $l_{blk}^{max} \simeq 1000$ sweeps



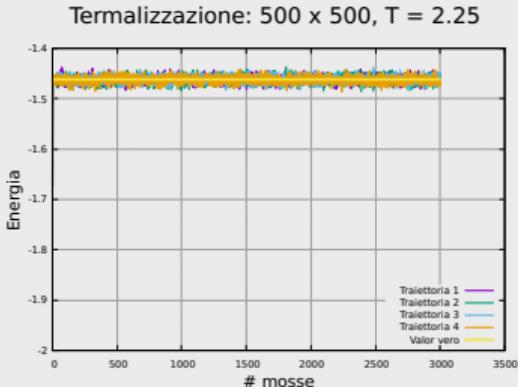


Caratterizzazione con Wolff

4 Simulazioni modello di Ising 2D

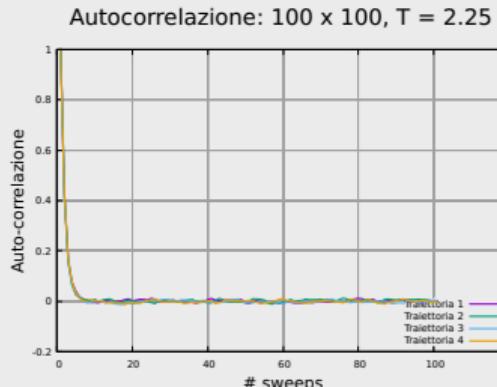
Termalizzazione

- ◊ Istantanea
- ◊ $t_{ter}^{max} \simeq 10$ sweeps



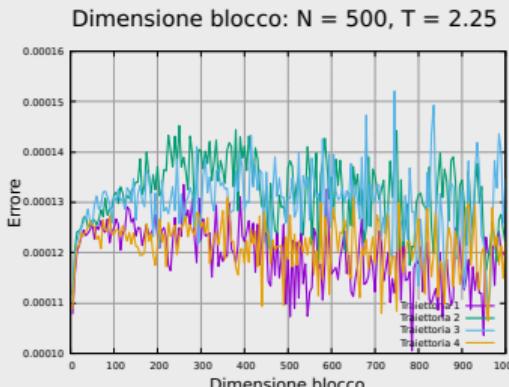
Auto-correlazione

- ◊ t_c maggiori per $T \simeq T_c$
- ◊ $t_c^{max} \simeq 40$ sweeps



Blocchi

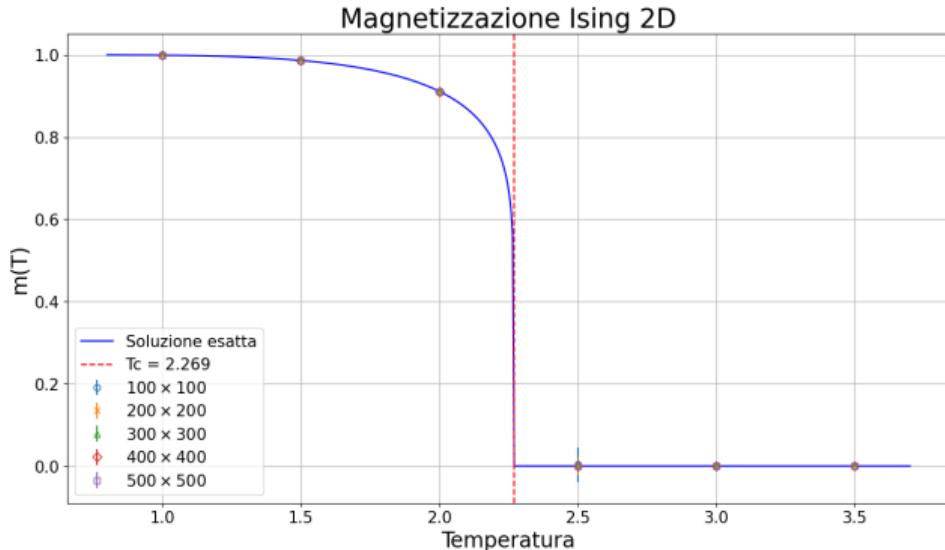
- ◊ l_{blk} maggiori per $T \simeq T_c$
- ◊ $l_{blk}^{max} \simeq 50$ sweeps



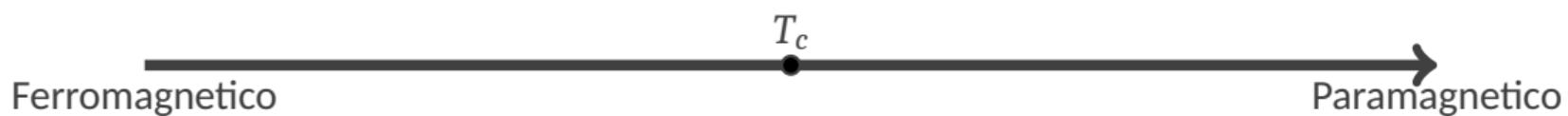


Magnetizzazione

4 Simulazioni modello di Ising 2D



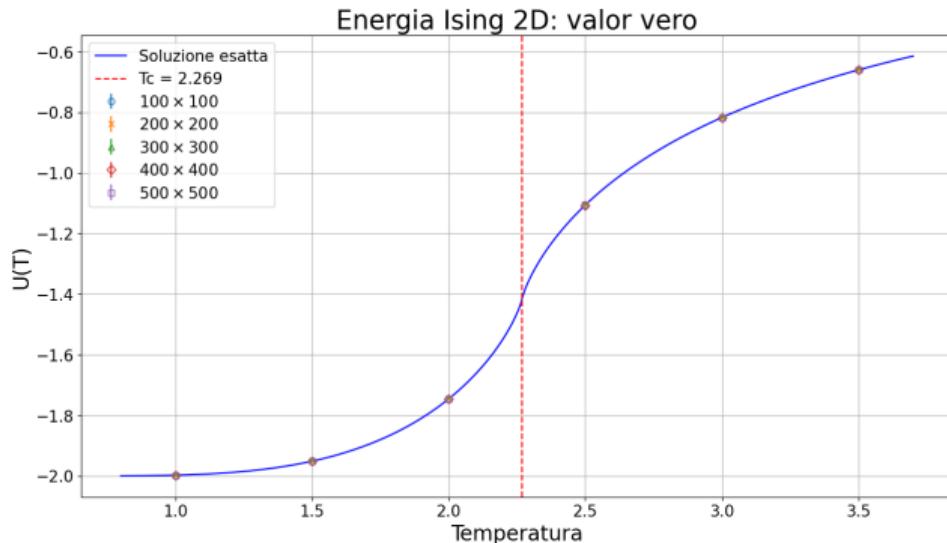
- ◊ Magnetizzazione spontanea per $T < T_c$
- ◊ Transizione di fase a T_c





Energia

4 Simulazioni modello di Ising 2D



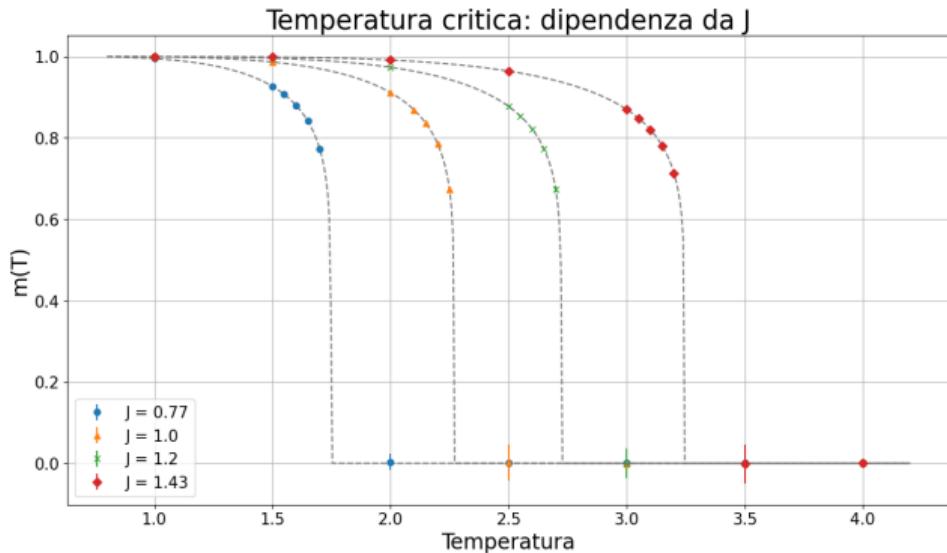
- ◊ copro tutto il reticolo con due legami per spin
- ◊ picco del calore specifico a T_c

$$U = -NJ \coth(2\beta J) \left\{ 1 + \frac{2}{\pi} [2 \tanh^2(2\beta J) - 1] \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - k^2 \sin^2(\phi)}} \right\}$$



T_c : dipendenza da J

4 Simulazioni modello di Ising 2D

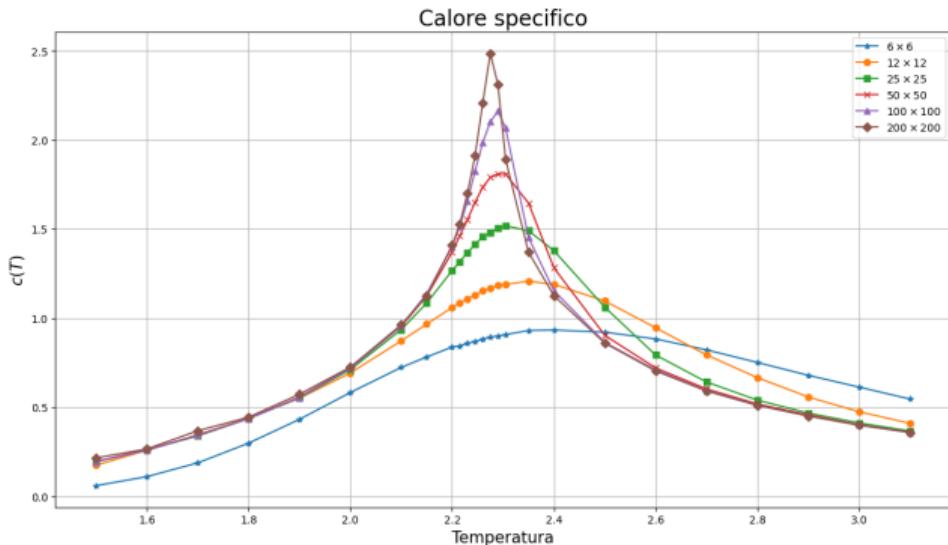


- ◊ Aumenta J , aumenta T_c
- ◊ Presenza o meno di ordine dipende dall'intensità dell'interazione



Regione critica

4 Simulazioni modello di Ising 2D

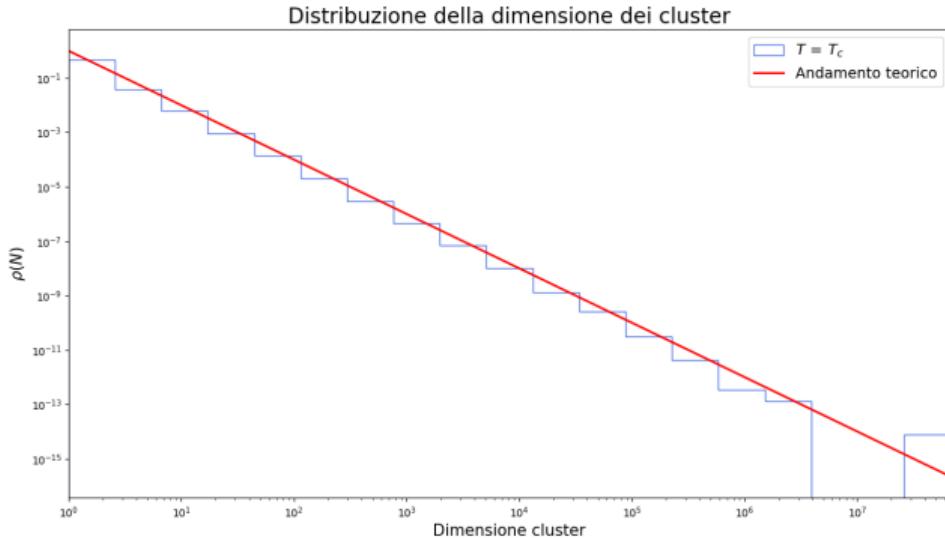


- ◊ Transizione di fase solo nel limite termodinamico
- ◊ Aumenta N , meglio risolto è il picco
- ◊ $N \rightarrow \infty$ implica $T_{max} \rightarrow T_c^+$

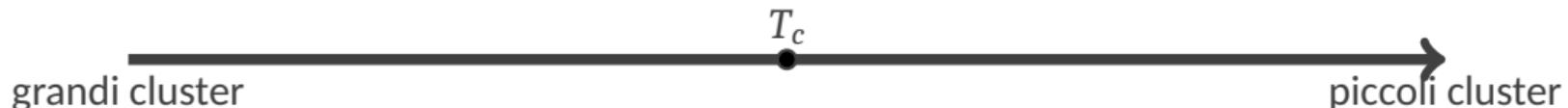


Dimensioni cluster

4 Simulazioni modello di Ising 2D



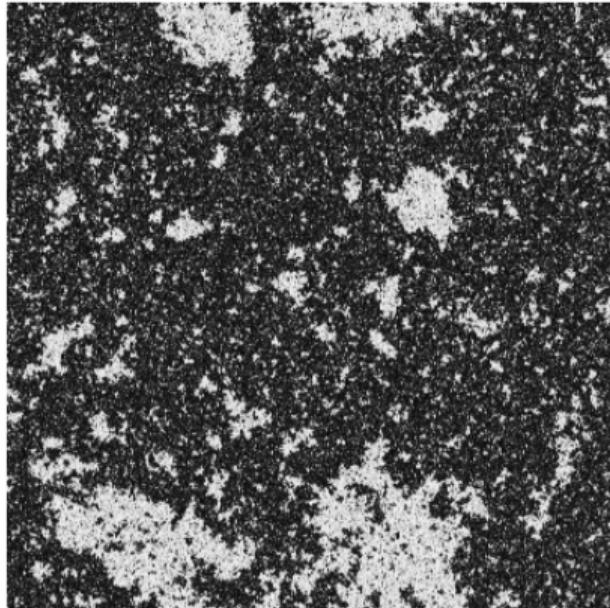
- ◊ $P(s) \propto s^{-\alpha}$
- ◊ $\alpha \simeq 2$
- ◊ perdita di un parametro di scala





Coarse graining

4 Simulazioni modello di Ising 2D



CG →

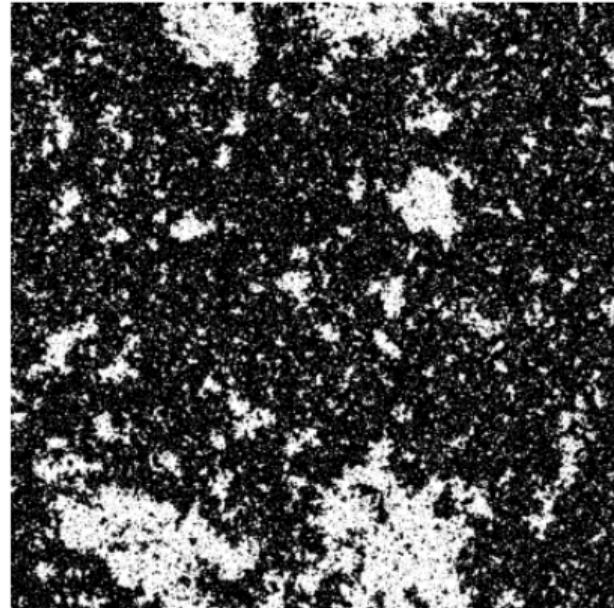




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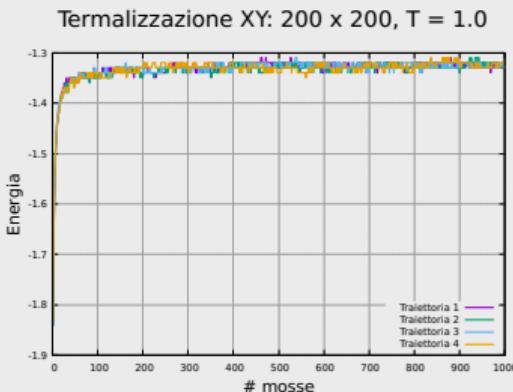


Caratterizzazione

5 Modello XY

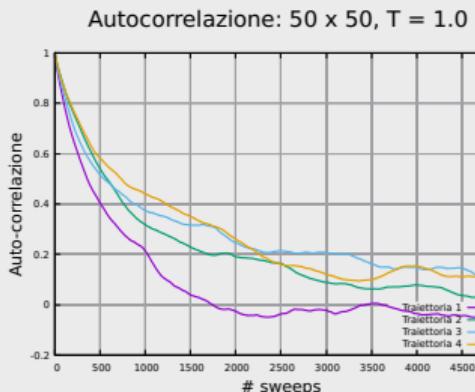
Termalizzazione

- ◊ t_{ter} maggiori per $T \rightarrow 0$
- ◊ $t_{ter}^{max} \simeq 300$ sweeps



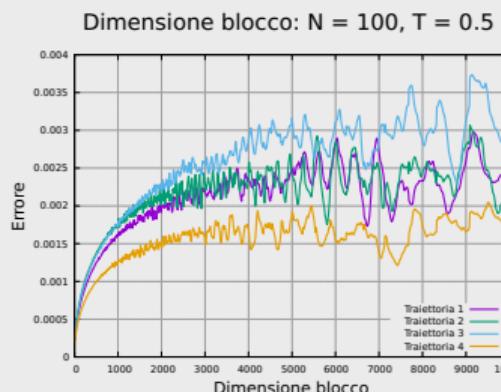
Auto-correlazione

- ◊ t_c maggiori per $T \rightarrow 0$
- ◊ $t_c^{max} \simeq 5000$ sweeps



Blocchi

- ◊ l_b maggiori per $T \rightarrow 0$
- ◊ $l_b^{max} \simeq 7000$ sweeps

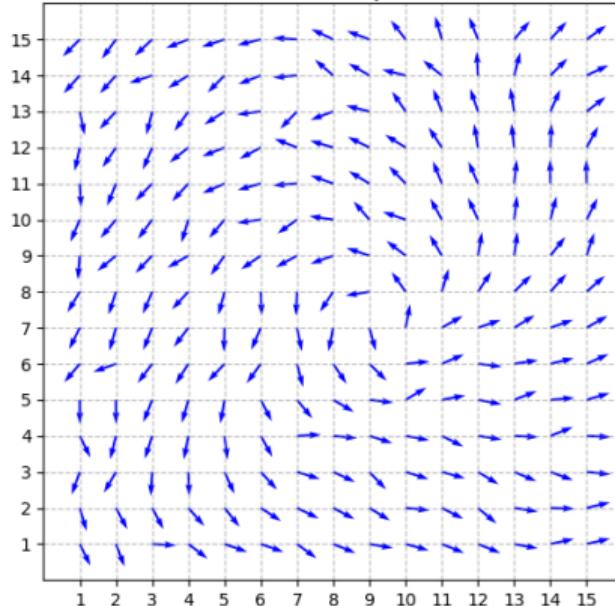




Vortice

5 Modello XY

Modello XY: esempio di vortice



- ◊ Winding number $w = 1$
- ◊ Transizione di Kosterlitz-Thouless

Temperatura critica

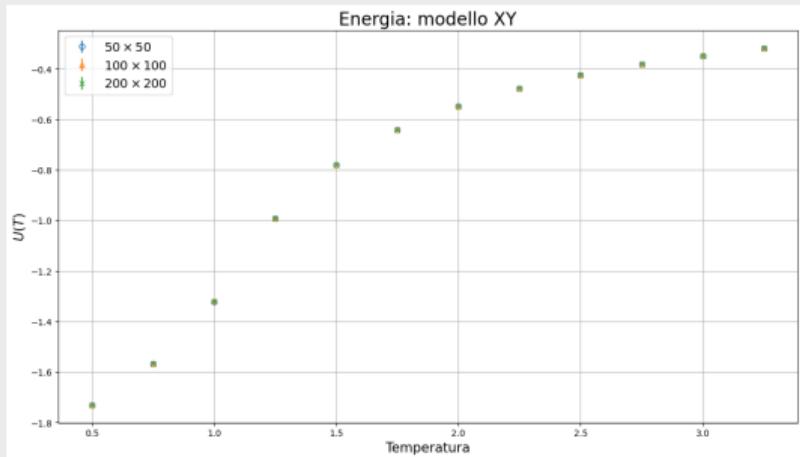
$$T_c = \frac{\pi J}{2}$$



Osservabili

5 Modello XY

Energia



Applicazione campo

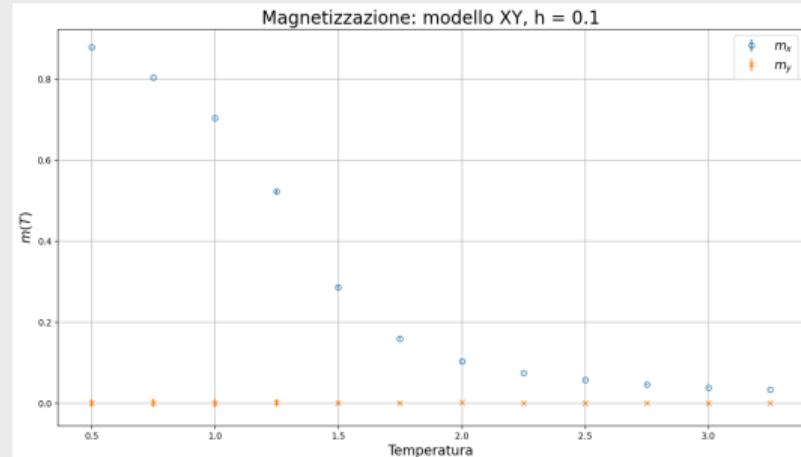




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Riassunto

6 Conclusioni

Ising 1D

- ◊ no fase ordinata con $h = 0.0$
- ◊ approccio MF fisicamente errato
- ◊ verifica criterio di Ginzburg

Ising 2D

- ◊ transizione di fase a $T_c \neq 0$
- ◊ modello ottimo per lo studio del punto critico
- ◊ rottura di simmetria discreta

Modello XY

- ◊ teorema di Mermin-Wagner
- ◊ transizione di fase topologica
- ◊ quasi long-range order per $T < T_{KT}$



Fine

6 Conclusioni

Grazie per l'attenzione



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7 Backup

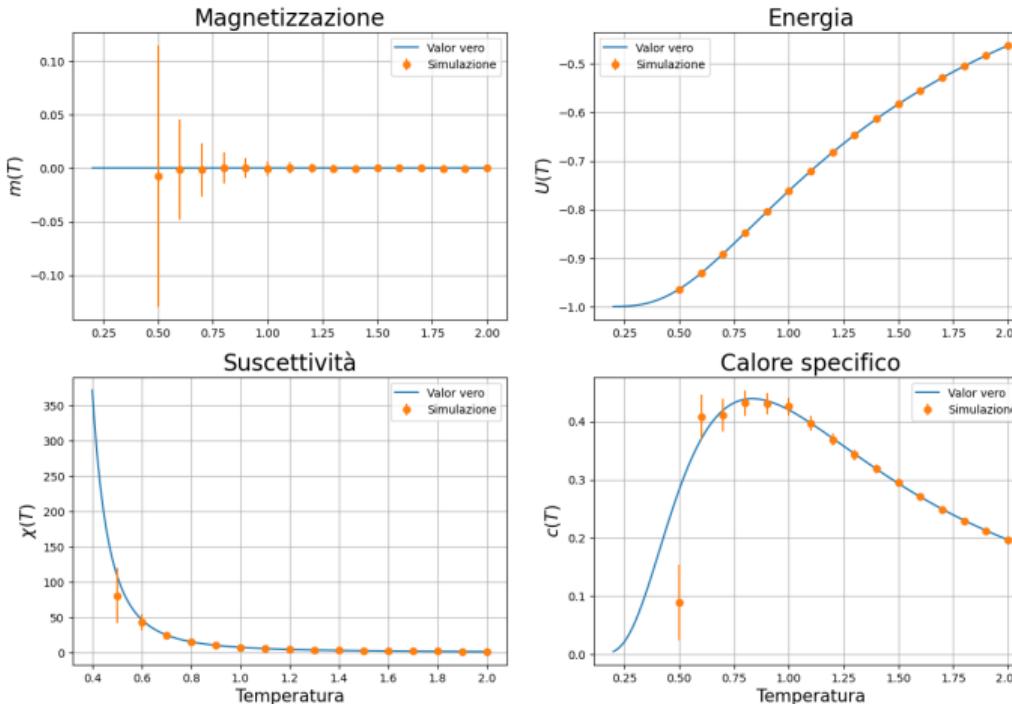
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Osservabili per $N_s = 1000$, $h = 0.0$

Ising 1D

Ising 1D: $N_s = 1000$, $h = 0.0$

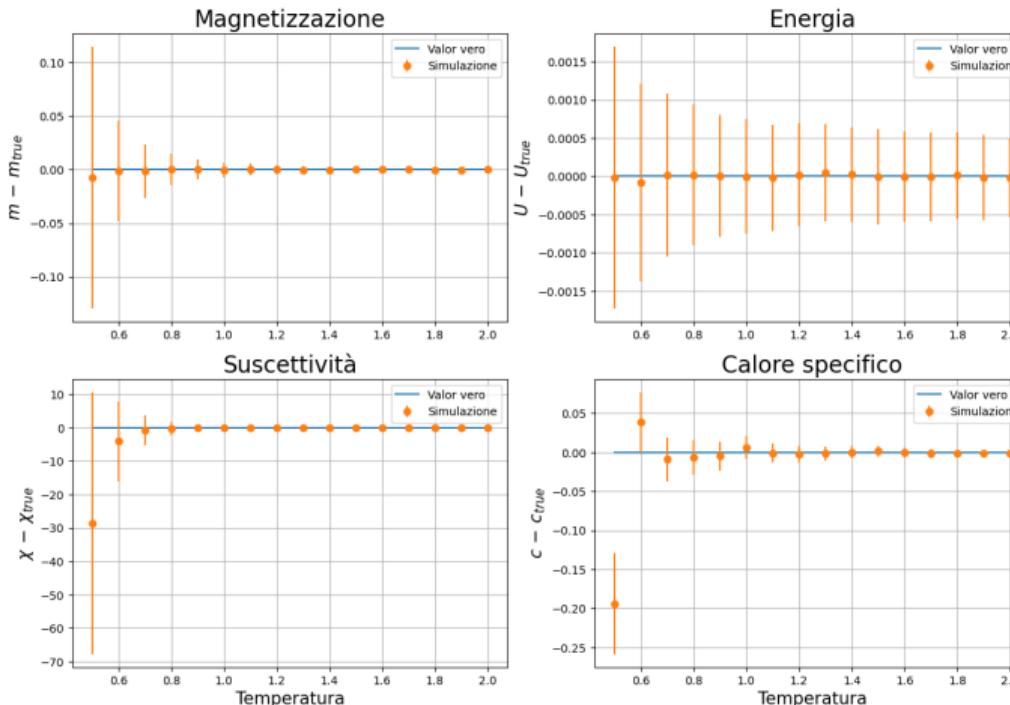




Differenza dal valor vero per $N_s = 1000$, $h = 0.0$

Ising 1D

Ising 1D: $N_s = 1000$, $h = 0.0$

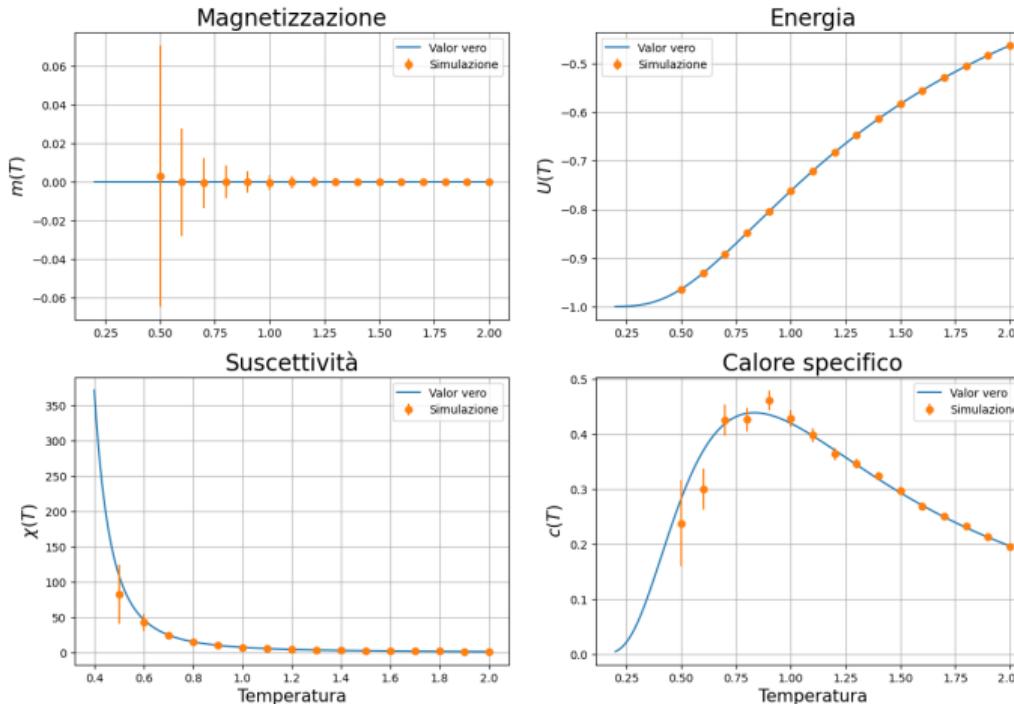




Osservabili per $N_s = 3000$, $h = 0.0$

Ising 1D

Ising 1D: $N_s = 3000$, $h = 0.0$

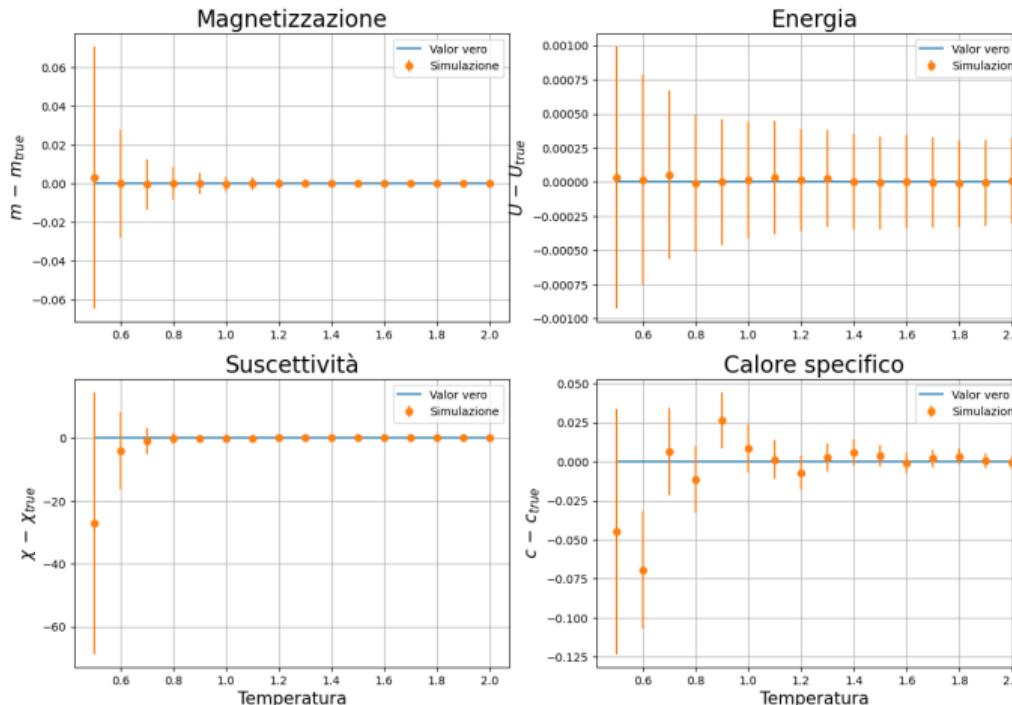




Differenza dal valor vero per $N_s = 3000$, $h = 0.0$

Ising 1D

Ising 1D: $N_s = 3000$, $h = 0.0$

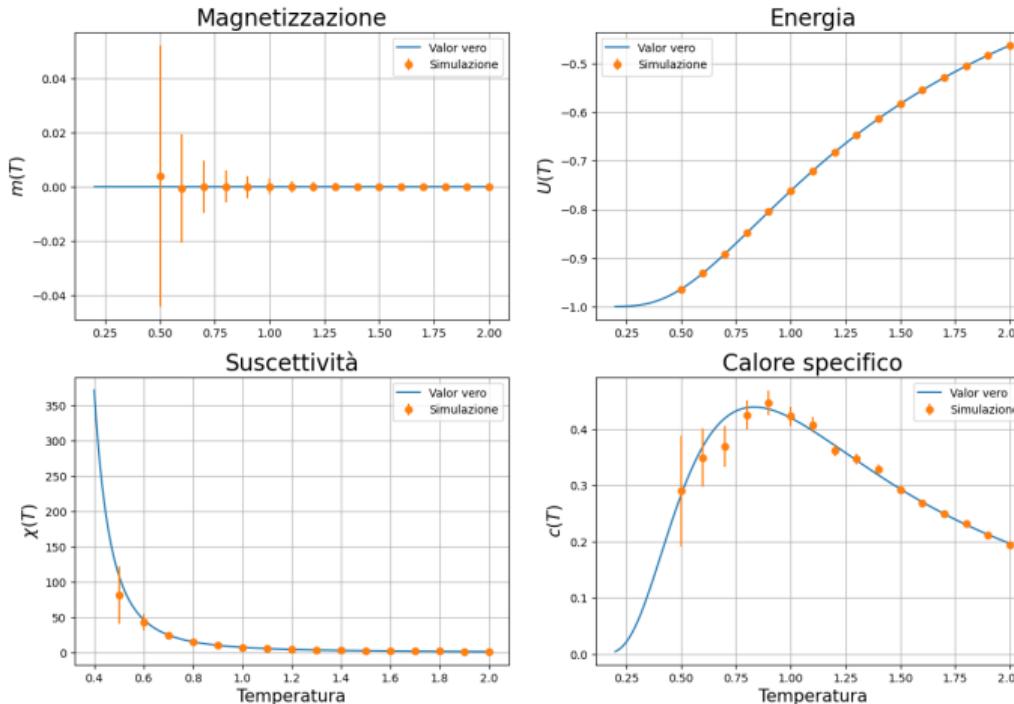




Osservabili per $N_s = 6000$, $h = 0.0$

Ising 1D

Ising 1D: $N_s = 6000$, $h = 0.0$

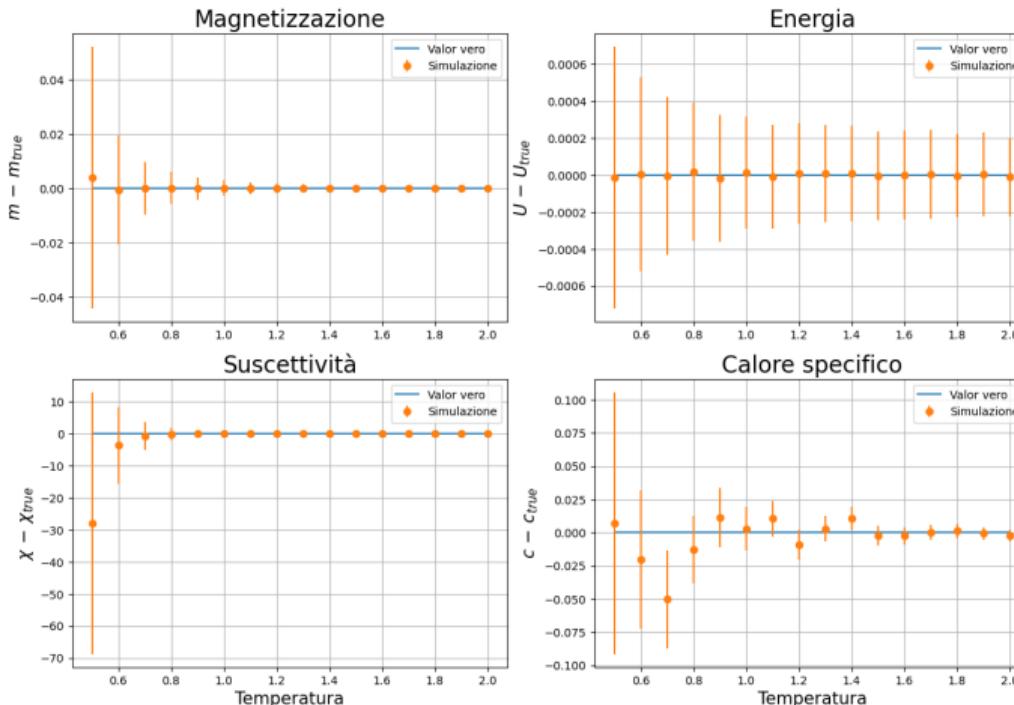




Differenza dal valor vero per $N_s = 6000$, $h = 0.0$

Ising 1D

Ising 1D: $N_s = 6000$, $h = 0.0$

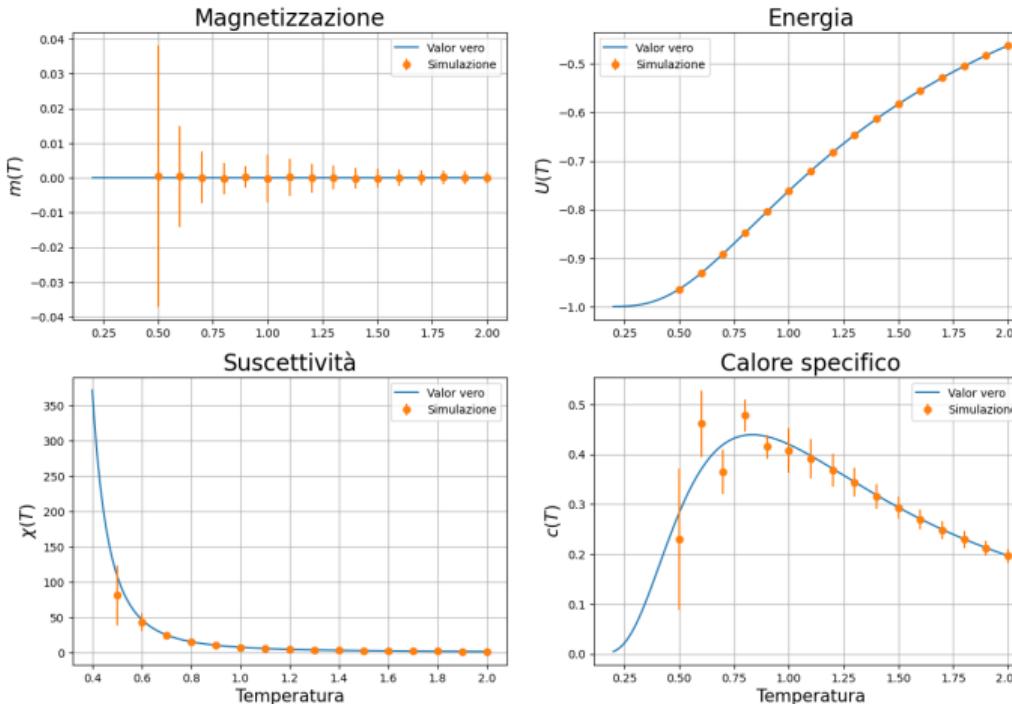




Osservabili per $N_s = 10000$, $h = 0.0$

Ising 1D

Ising 1D: $N_s = 10000$, $h = 0.0$

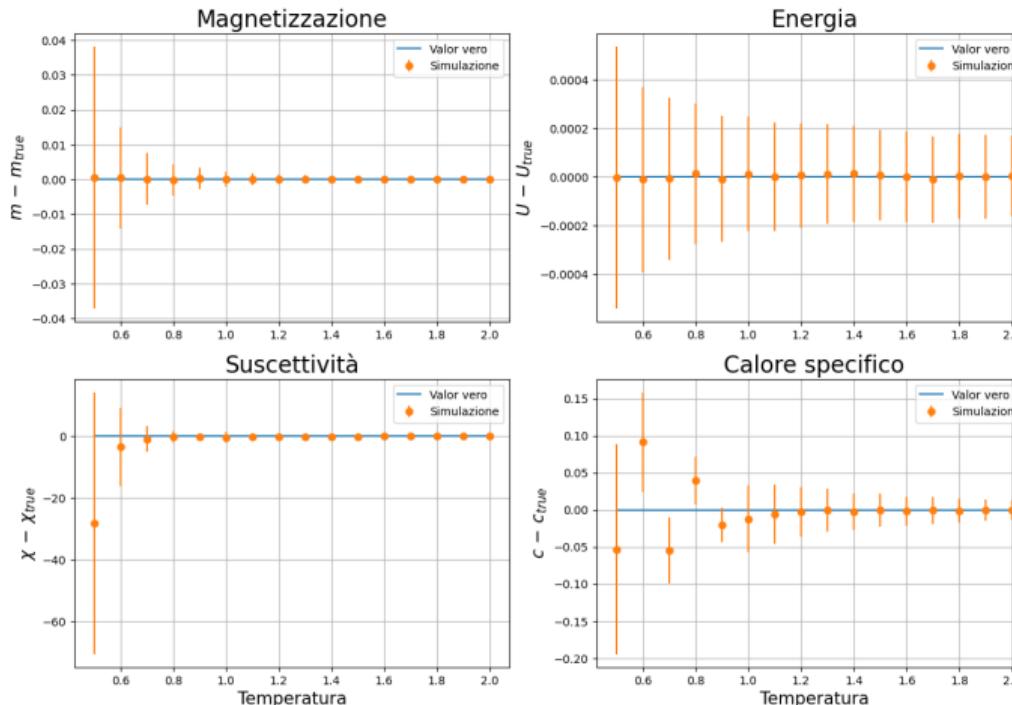




Differenza dal valor vero per $N_s = 10000$, $h = 0.0$

Ising 1D

Ising 1D: $N_s = 10000$, $h = 0.0$

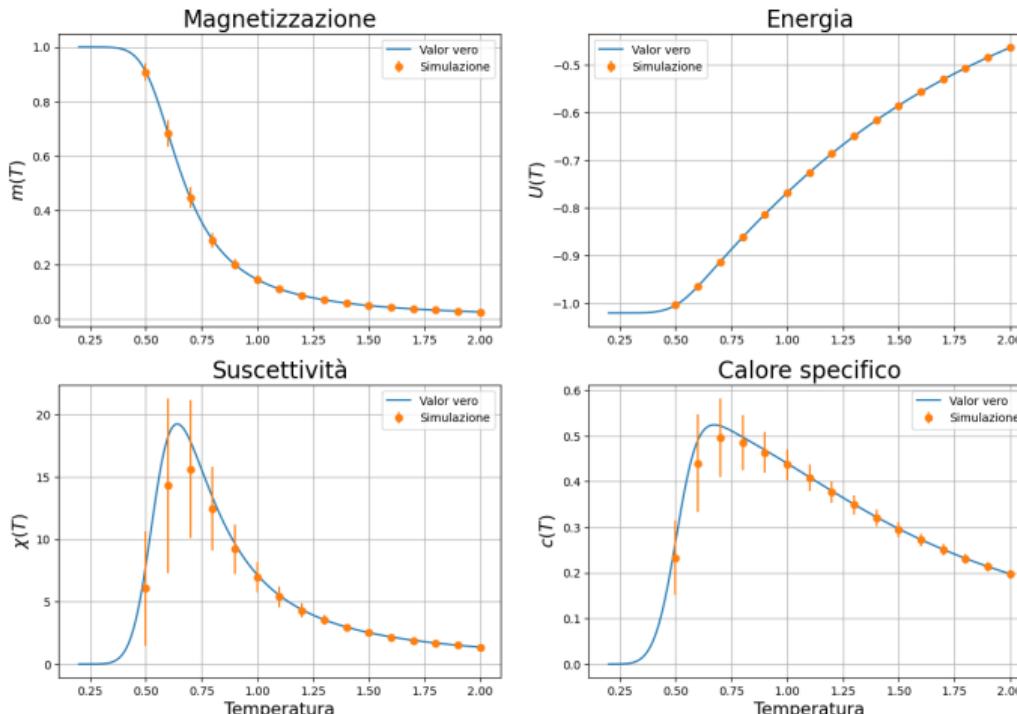




Osservabili per $N_s = 1000$, $h = 0.02$

Ising 1D

Ising 1D: $N_s = 1000$, $h = 0.02$

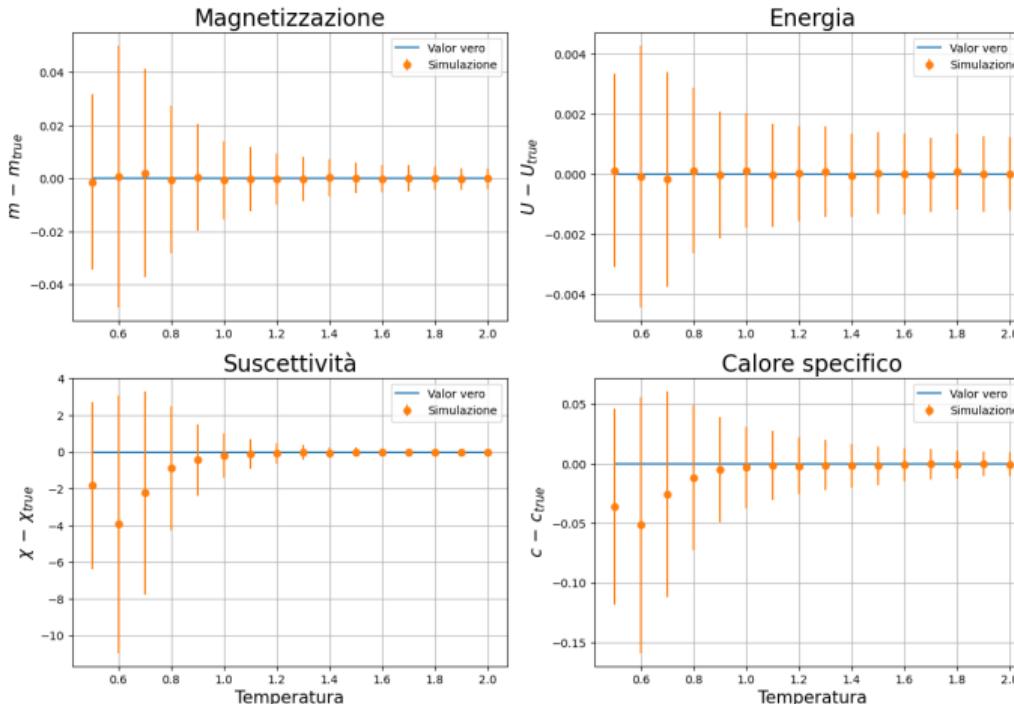




Differenza dal valor vero per $N_s = 1000$, $h = 0.02$

Ising 1D

Ising 1D: $N_s = 1000$, $h = 0.02$

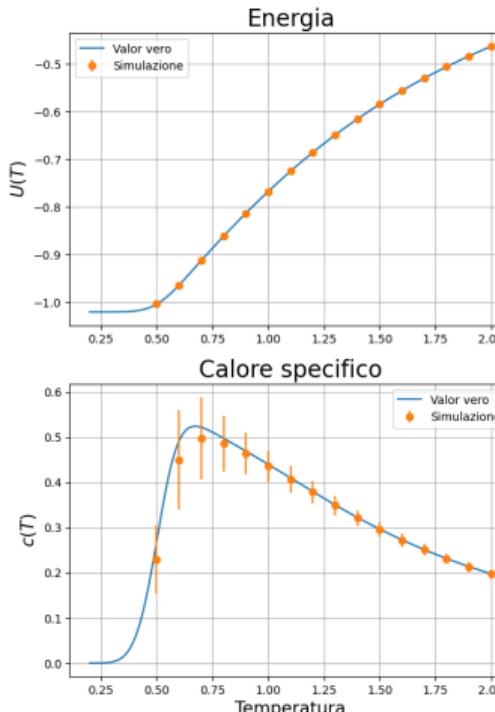
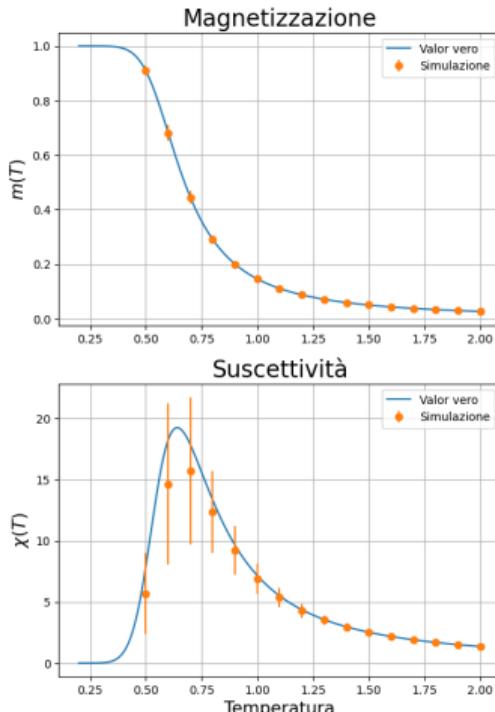




Osservabili per $N_s = 3000$, $h = 0.02$

Ising 1D

Ising 1D: $N_s = 3000$, $h = 0.02$

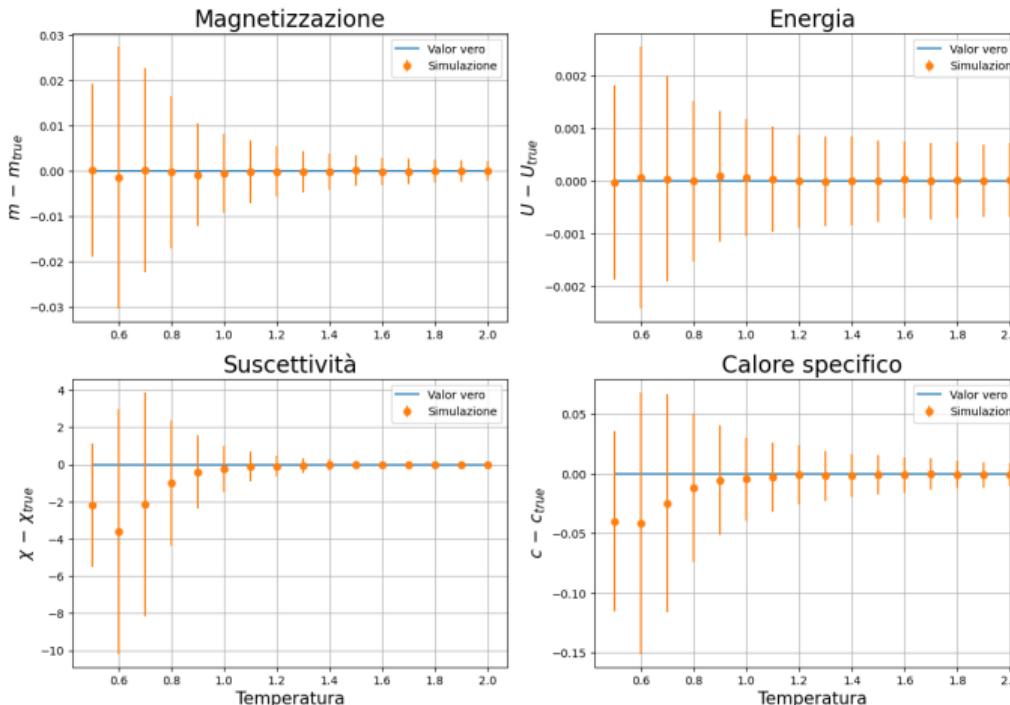




Differenza dal valor vero per $N_s = 3000$, $h = 0.02$

Ising 1D

Ising 1D: $N_s = 3000$, $h = 0.02$

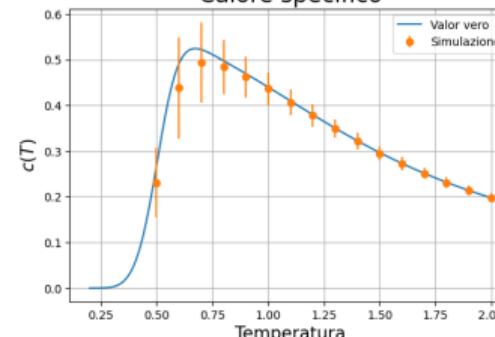
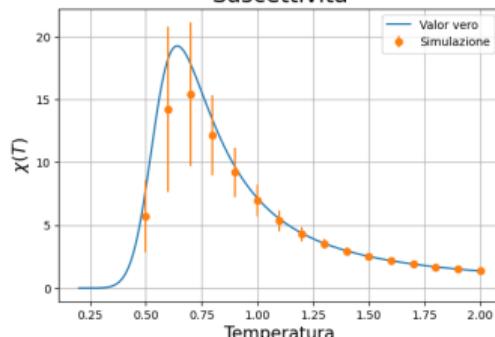
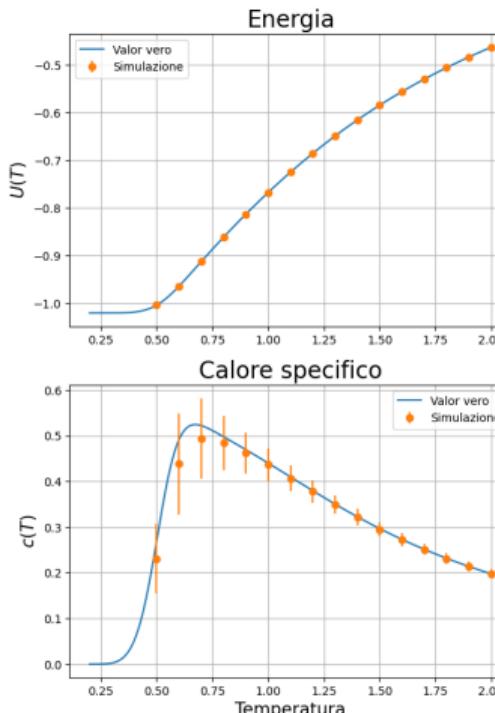
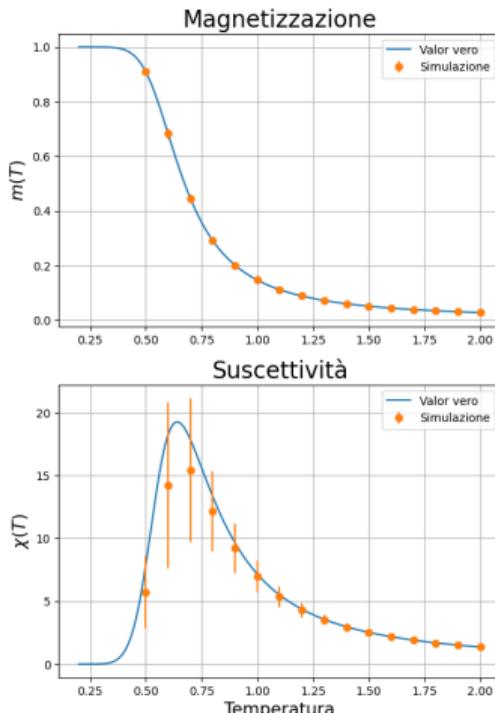




Osservabili per $N_s = 6000$, $h = 0.02$

Ising 1D

Ising 1D: $N_s = 6000$, $h = 0.02$

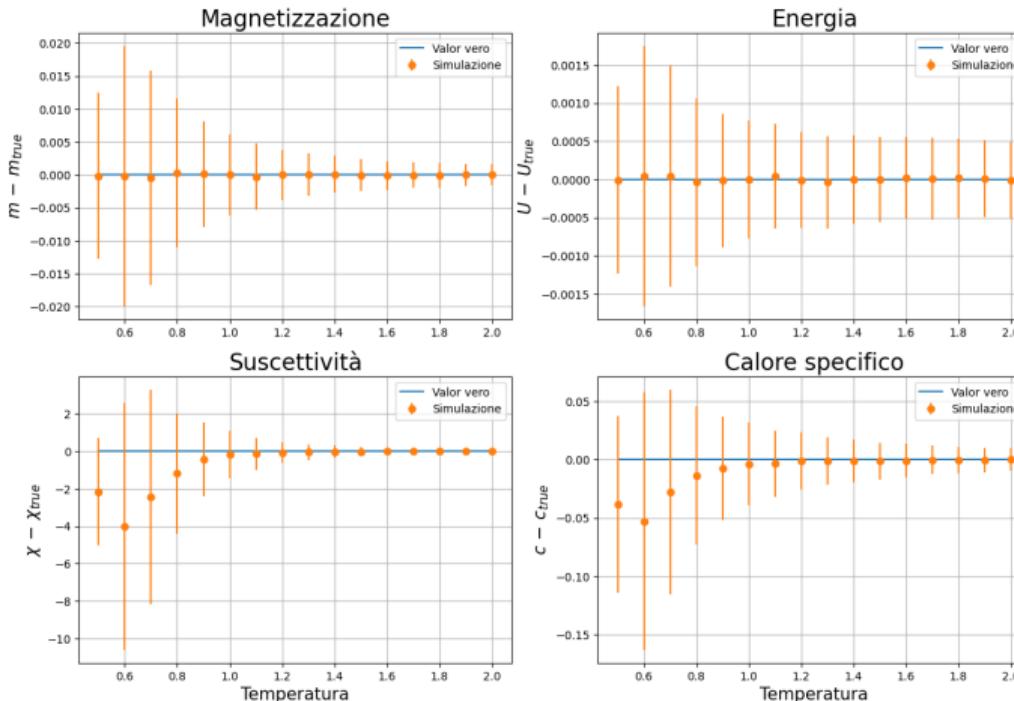




Differenza dal valor vero per $N_s = 6000$, $h = 0.02$

Ising 1D

Ising 1D: $N_s = 6000$, $h = 0.02$

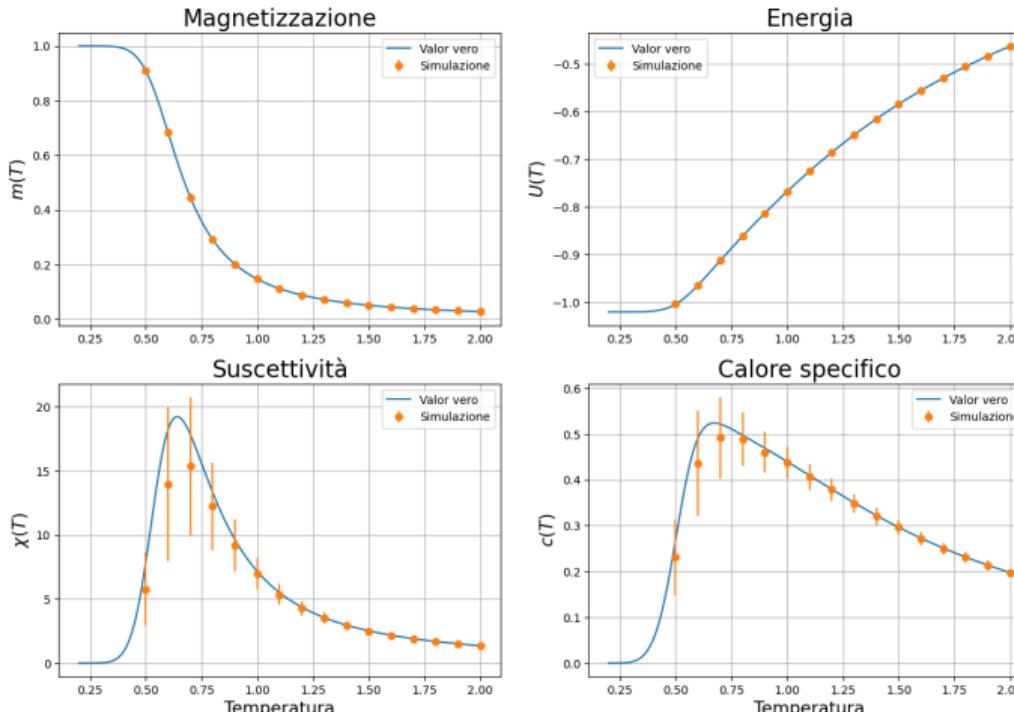




Osservabili per $N_s = 10000$, $h = 0.02$

Ising 1D

Ising 1D: $N_s = 10000$, $h = 0.02$

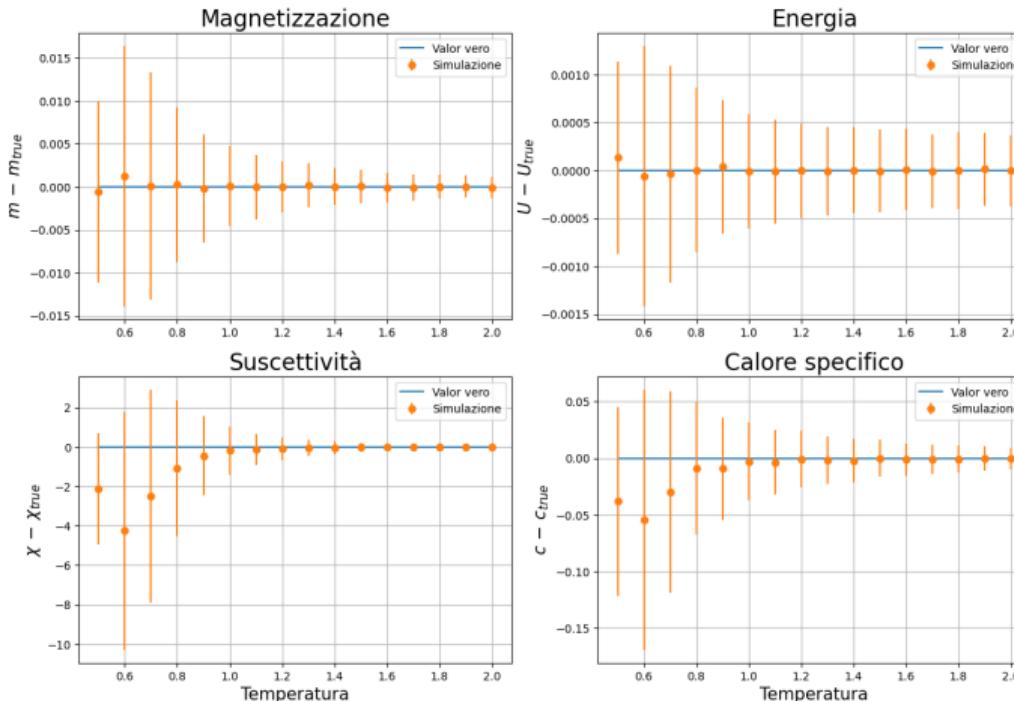




Differenza dal valor vero per $N_s = 10000$, $h = 0.02$

Ising 1D

Ising 1D: $N_s = 10000$, $h = 0.02$

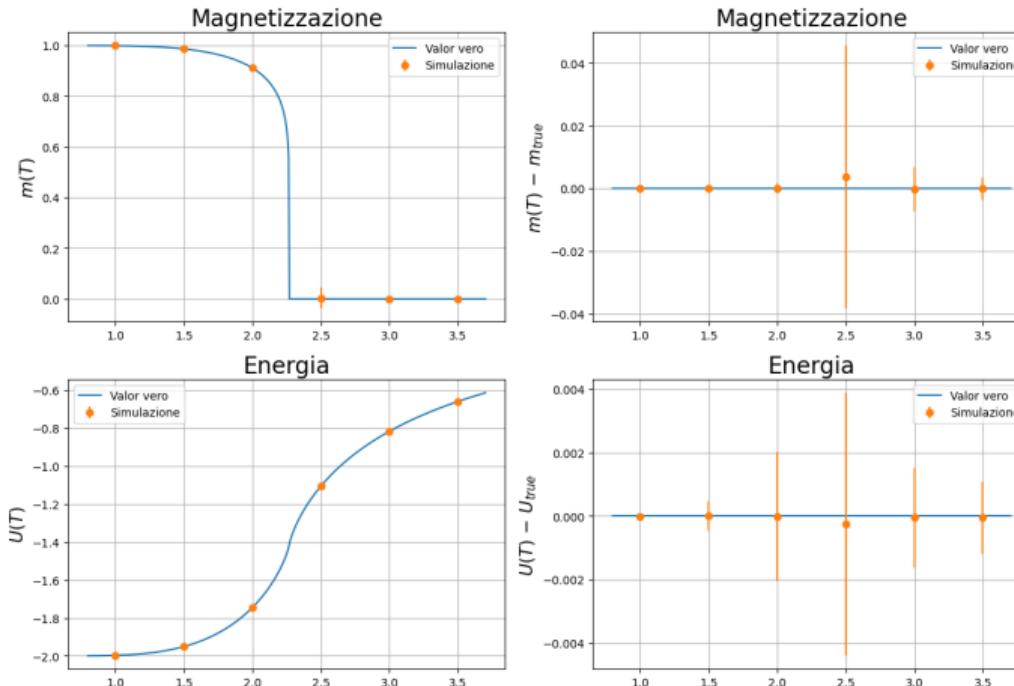




Osservabili per reticolo 100×100

Ising 2D

Ising 2D: reticolo 100×100

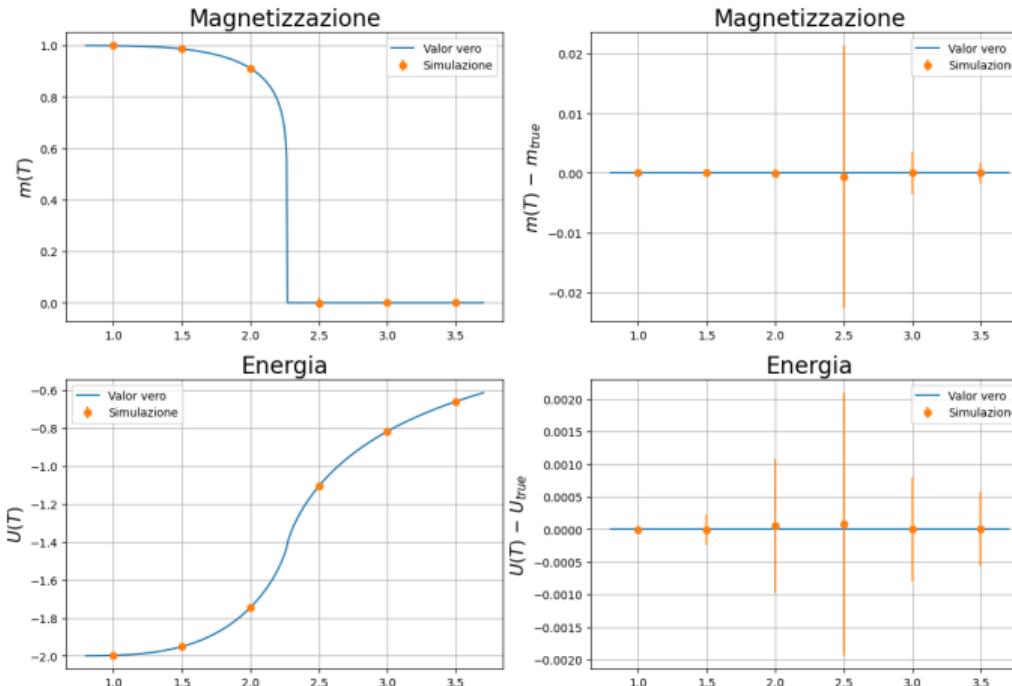




Osservabili per reticolo 200×200

Ising 2D

Ising 2D: reticolo 200×200

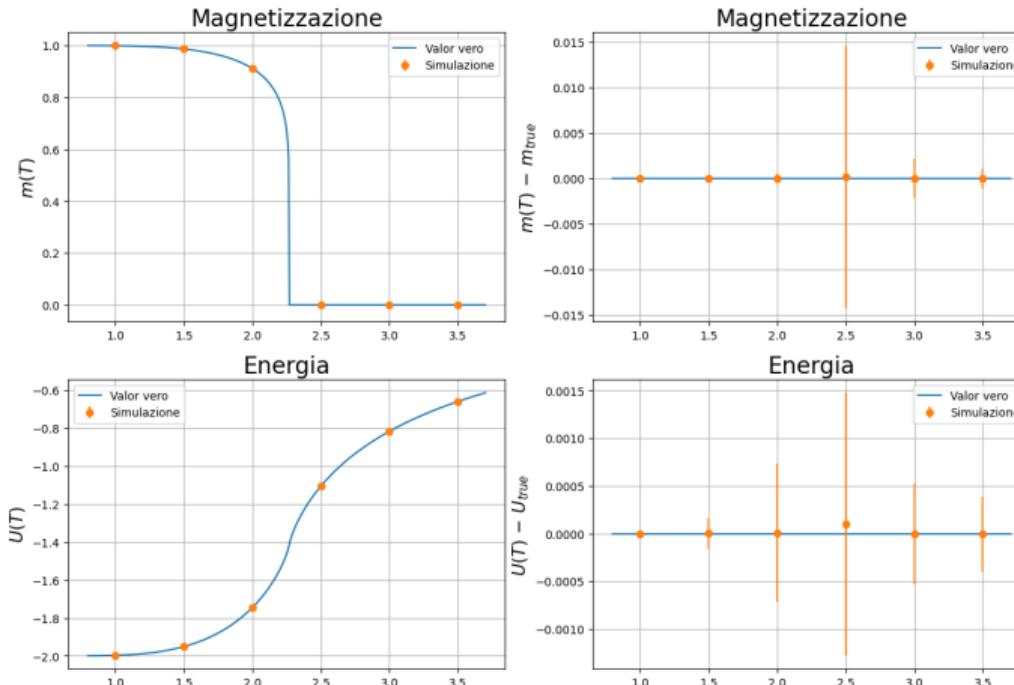




Osservabili per reticolo 300×300

Ising 2D

Ising 2D: reticolo 300×300

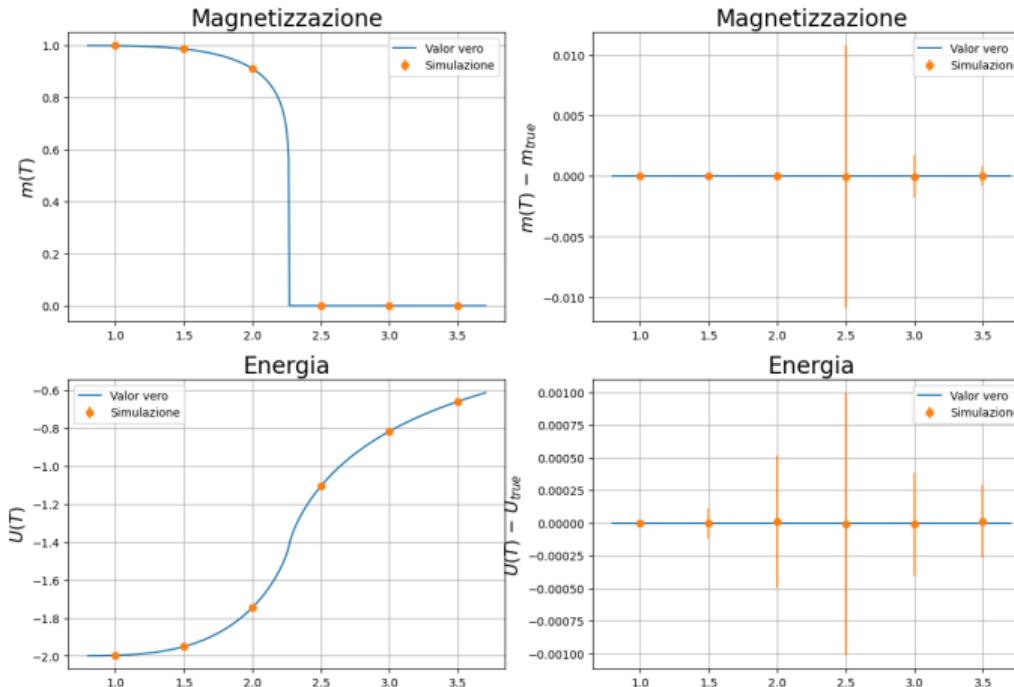




Osservabili per reticolo 400×400

Ising 2D

Ising 2D: reticolo 400×400

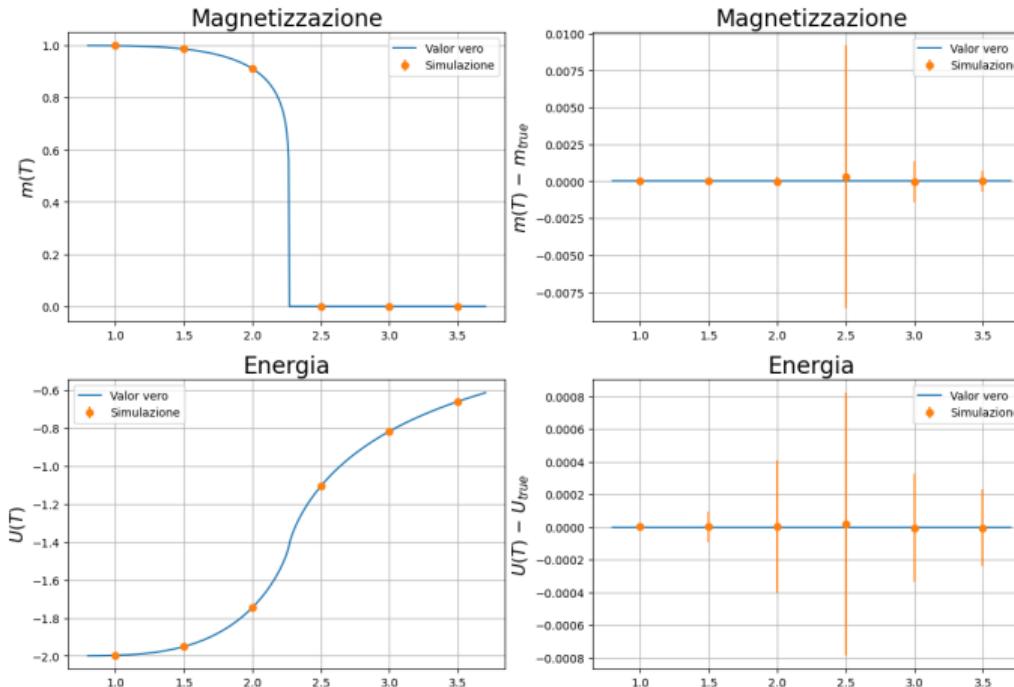




Osservabili per reticolo 500×500

Ising 2D

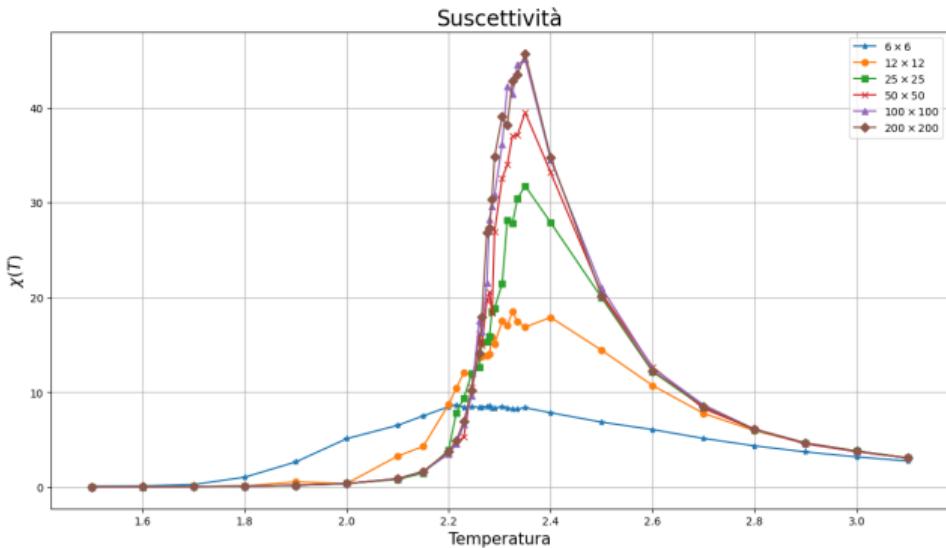
Ising 2D: reticolo 500×500





Suscettività

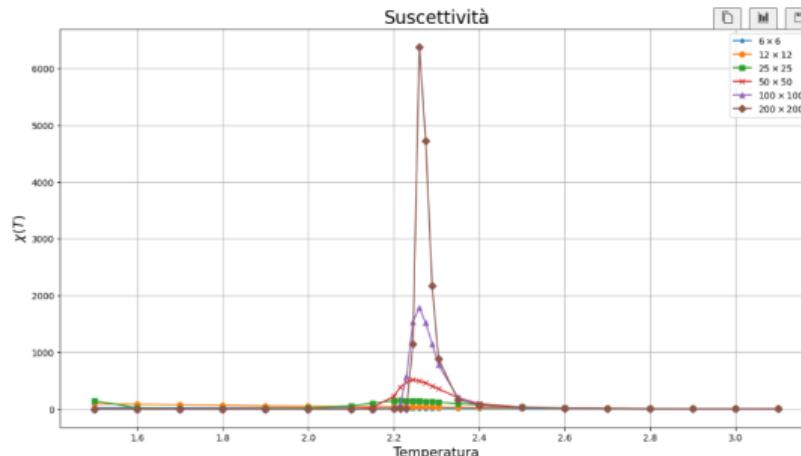
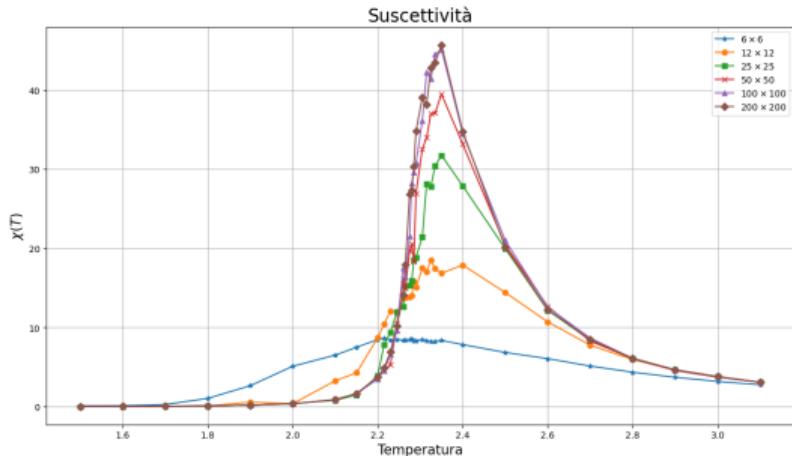
Ising 2D



- ◊ Transizione di fase solo nel limite termodinamico
- ◊ Aumenta N , meglio risolto è il picco
- ◊ $N \rightarrow \infty$ implica $T_{max} \rightarrow T_c^+$

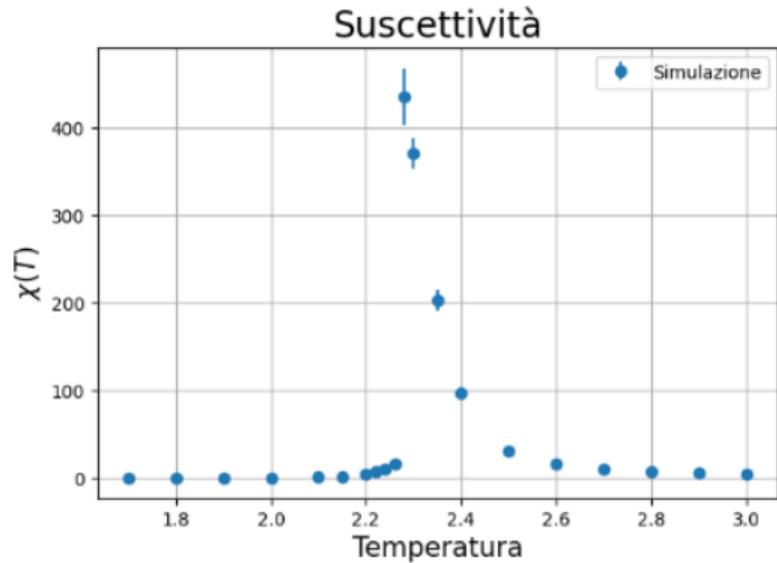
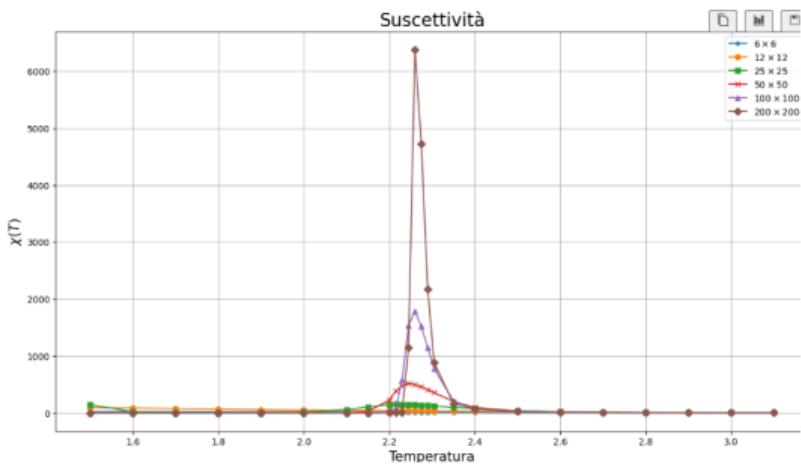


Suscettività: Metropolis vs Wolff Ising 2D





Suscettività: confronto Wolff Ising 2D



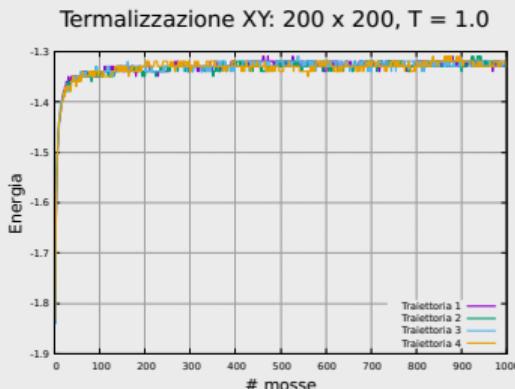


Caratterizzazione Metropolis

Modello XY

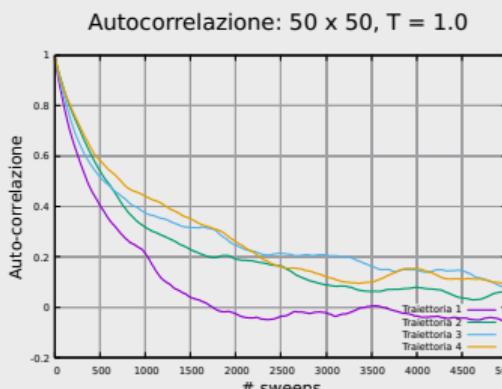
Termalizzazione

- ◊ t_t maggiori per $T \rightarrow T_{KT}$
- ◊ $t_t^{max} \simeq 200$ sweeps



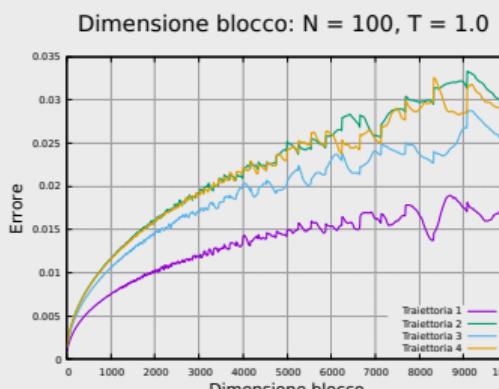
Auto-correlazione

- ◊ t_c maggiori per $T \rightarrow T_{KT}^-$
- ◊ $t_c^{max} \simeq 5000$ sweeps



Blocchi

- ◊ l_b maggiori per $T \rightarrow T_{KT}^-$
- ◊ $l_b^{max} \simeq 10000$ sweeps



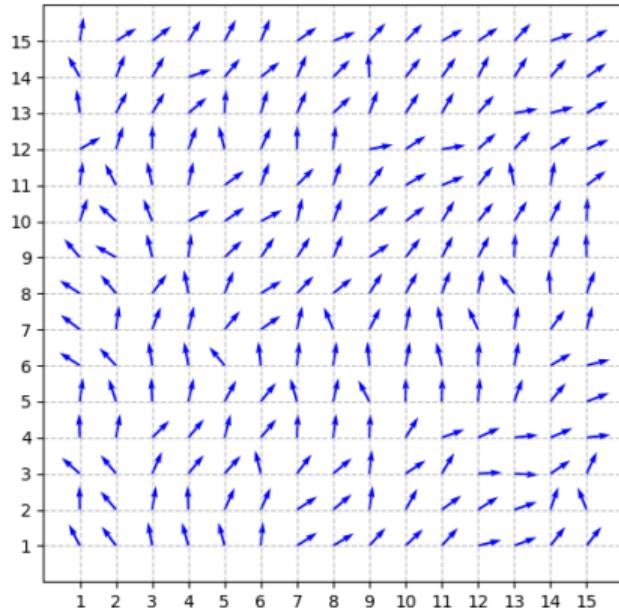


Configurazioni

ModelloXY

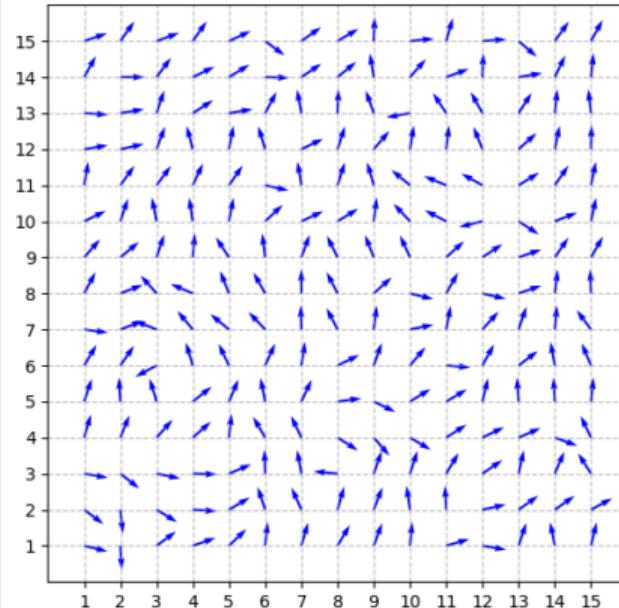
$T = 0.5$

Modello XY: $T = 0.5$



$T = 1.0$

Modello XY: $T = 1.0$



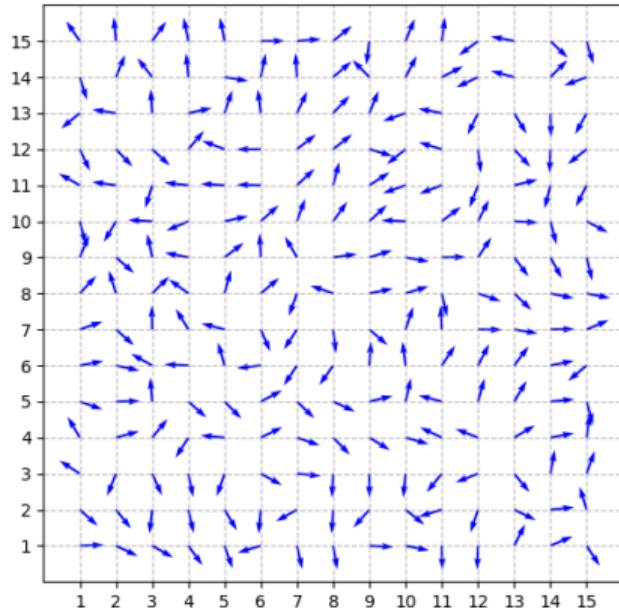


Configurazioni

Modello XY

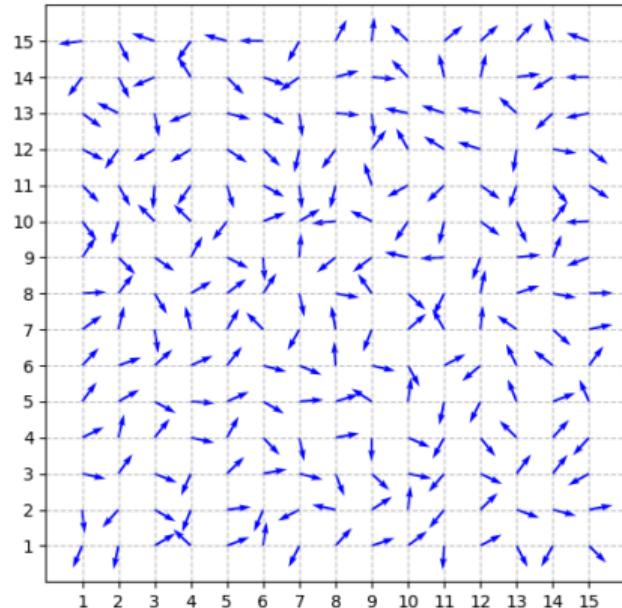
$T = 1.5$

Modello XY: $T = 1.5$



$T = 2.0$

Modello XY: $T = 2.0$



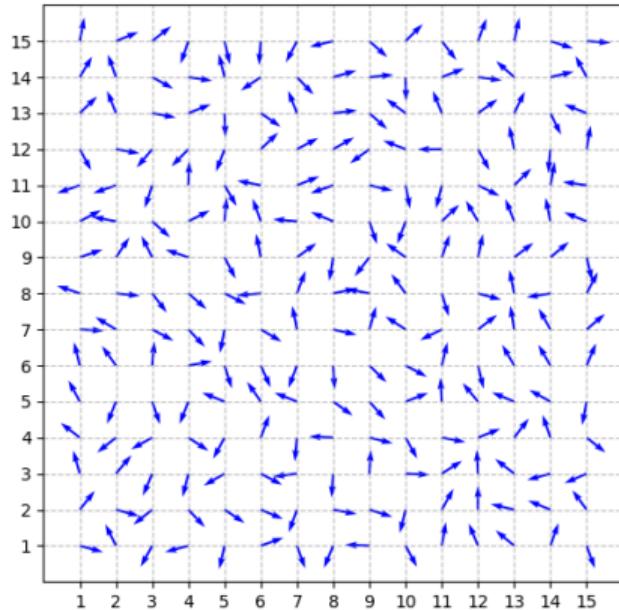


Configurazioni

Modello XY

$T = 2.5$

Modello XY: $T = 2.5$



$T = 3.0$

Modello XY: $T = 3.0$

