Алгоритм «Population Annealing» и его применение к двумерным моделям Изинга и Поттса

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Population annealing

Инициализация. $\beta = 0 \;\; (T = \infty)$. Каждая реплика находится в случайно выбранном микросостоянии.

Перевыборка (resampling). Температуру множества реплик понижаем, оставляя ансамбль в равновесии. Рассмотрим переход $1/\beta \Rightarrow 1/\beta'$ для $\tilde{R}_\beta$ реплик. Число копий состояния j в новой популяции есть $\mathcal{N}[(R_{\beta'}/\tilde{R}_\beta)\tau_j(\beta,\beta')]$, где

$$\tau_j(\beta,\beta') = \frac{\exp[-(\beta'-\beta)E_j]}{Q(\beta,\beta')}, \qquad Q(\beta,\beta') = \frac{1}{\tilde{R}_\beta}\sum_{j=1}^{\tilde{R}_\beta} \exp[-(\beta'-\beta)E_j].$$

Здесь $\mathcal{N}[a]$ – случайная целая величина с пуассоновским распределением и средним значением a. (Наряду с poisson resampling, существуют версии алгоритма с multinomial resampling, residual resampling, nearest integer resampling). Если $\mathcal{N}[(R_{\beta'}/\tilde{R}_\beta)\tau_j(\beta,\beta')] = 0$, то конфигурация j уничтожается.

Уравновешивание (equilibration). Для каждой реплики производится θ проходов сетки алгоритмом Монте-Карло (Monte-Carlo sweeps).

Population annealing

Инициализируем R_0 реплик для $\beta = 0$.

```
for k = K to 1 step -1 do
```

вычисляем отношение стат. сумм $Q(\beta_k, \beta_{k-1})$

`for all` $j \le \tilde{R}_{\beta_k}$ `do`

Вычисляем весовую функцию $\tau_j(\beta_k, \beta_{k-1})$

Перевыборка: создаем $\mathcal{N}[(R_{\beta'}/\tilde{R}_\beta)\tau_j(\beta, \beta')]$ копий реплики j

`end for`

Вычисляем новый размер популяции $\tilde{R}_{\beta_{k-1}}$

`for all` $j \le \tilde{R}_{\beta_{k-1}}$ `do`

Уравновешивание реплики j: производим θ_{k-1} проходов Монте-Карло

`end for`

Вычисляем наблюдаемые величины и свободную энергию для β_{k-1}

`end for`

Свободная энергия: $-\beta_k \tilde{F}(\beta_k) = \sum_{l=k}^{k+1} \ln Q(\beta_l, \beta_{l-1}) + \ln \Omega$,
где $Q(\beta, \beta') \approx Z(\beta')/Z(\beta)$ было вычислено ранее.
Взвешенные средние по результатам M независимых запусков программы:
$\langle A(\beta) \rangle = \sum_{r=1}^{M} \tilde{A}_r(\beta)\omega_r(\beta)$, где $\omega_r(\beta) = \frac{\exp(-\beta \tilde{F}_r(\beta))}{\sum_{r=1}^{M} \exp(-\beta \tilde{F}_r(\beta))}$.

Population annealing, 2D Ising model on the square lattice, L = 32

Effect of equilibration

$R = 10^3$, weighted average over $M = 200$ independent runs, $\Delta\beta = 0.001$

(CUDA algorithm was tested by M. Borovsky and by L.Barash)

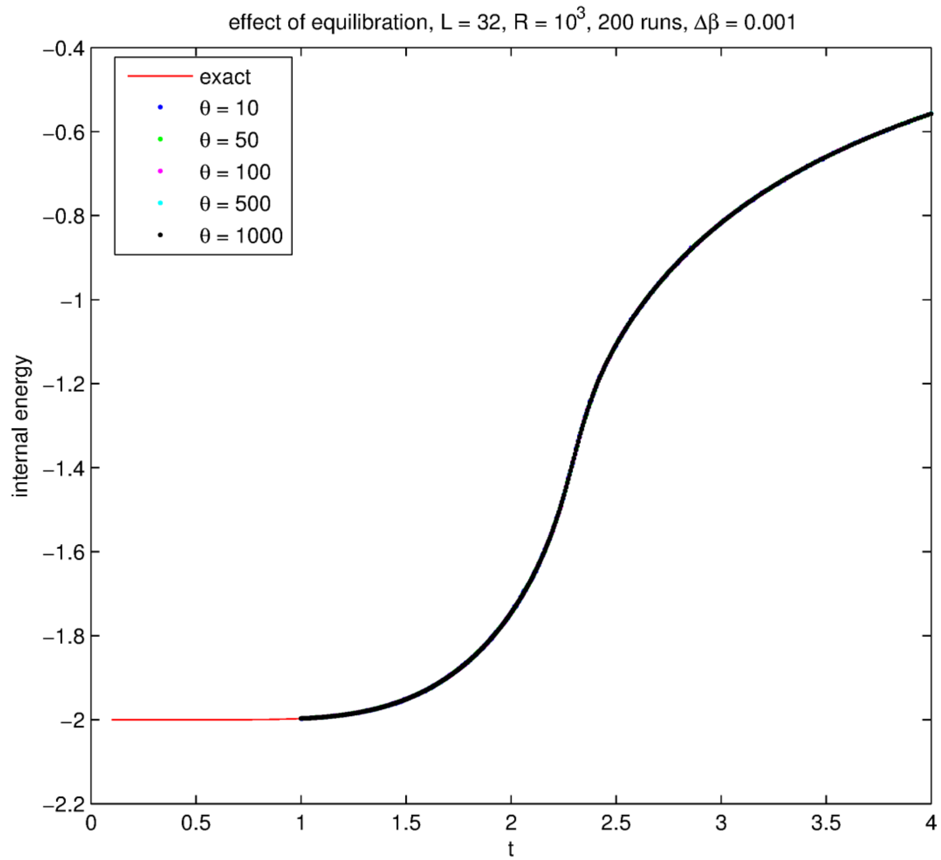


Figure 1: Internal energy per spin as a function of the temperature $t = k_B T/J$ for a different number of equilibration sweeps θ.

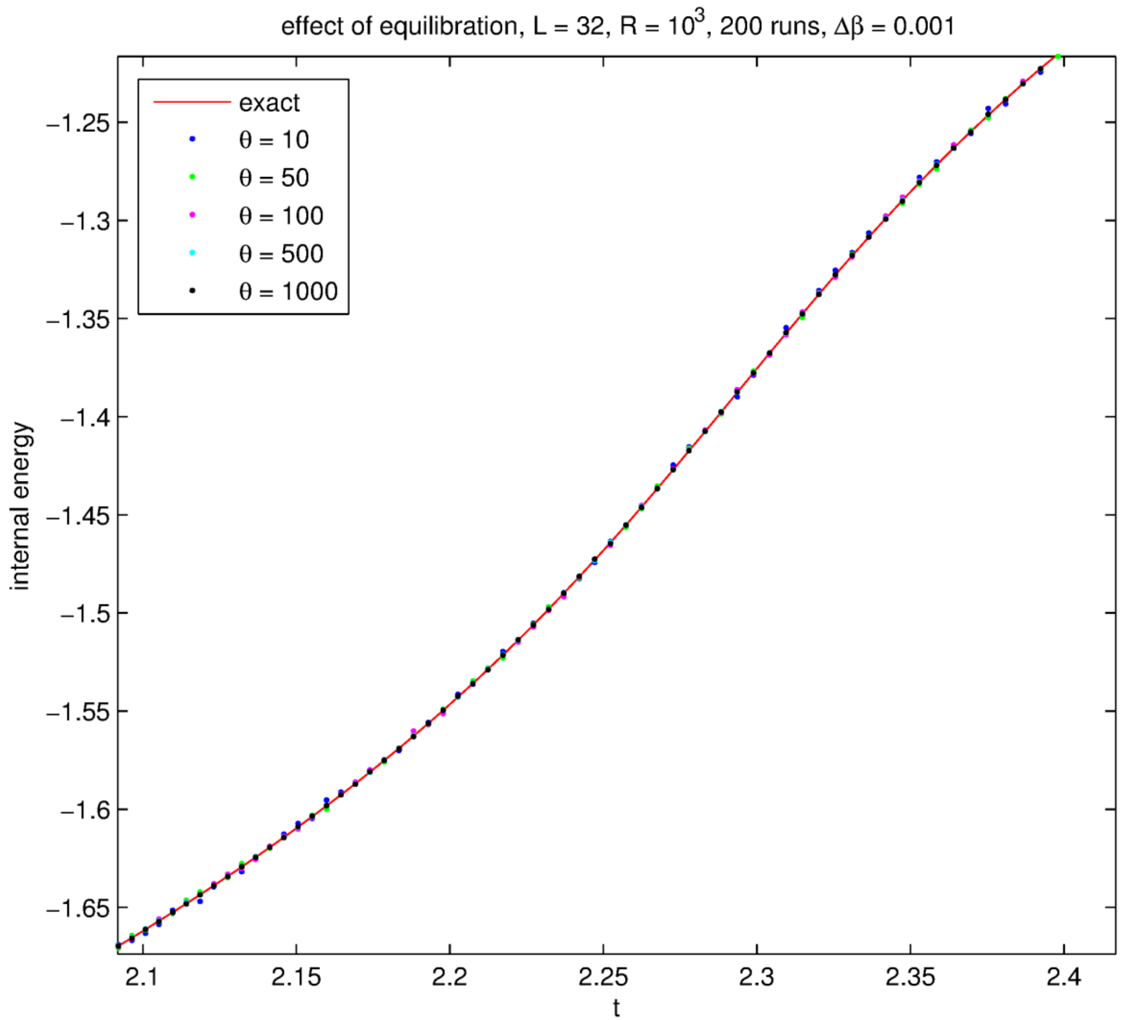


Figure 2: Detail from the previous plot in the critical region.

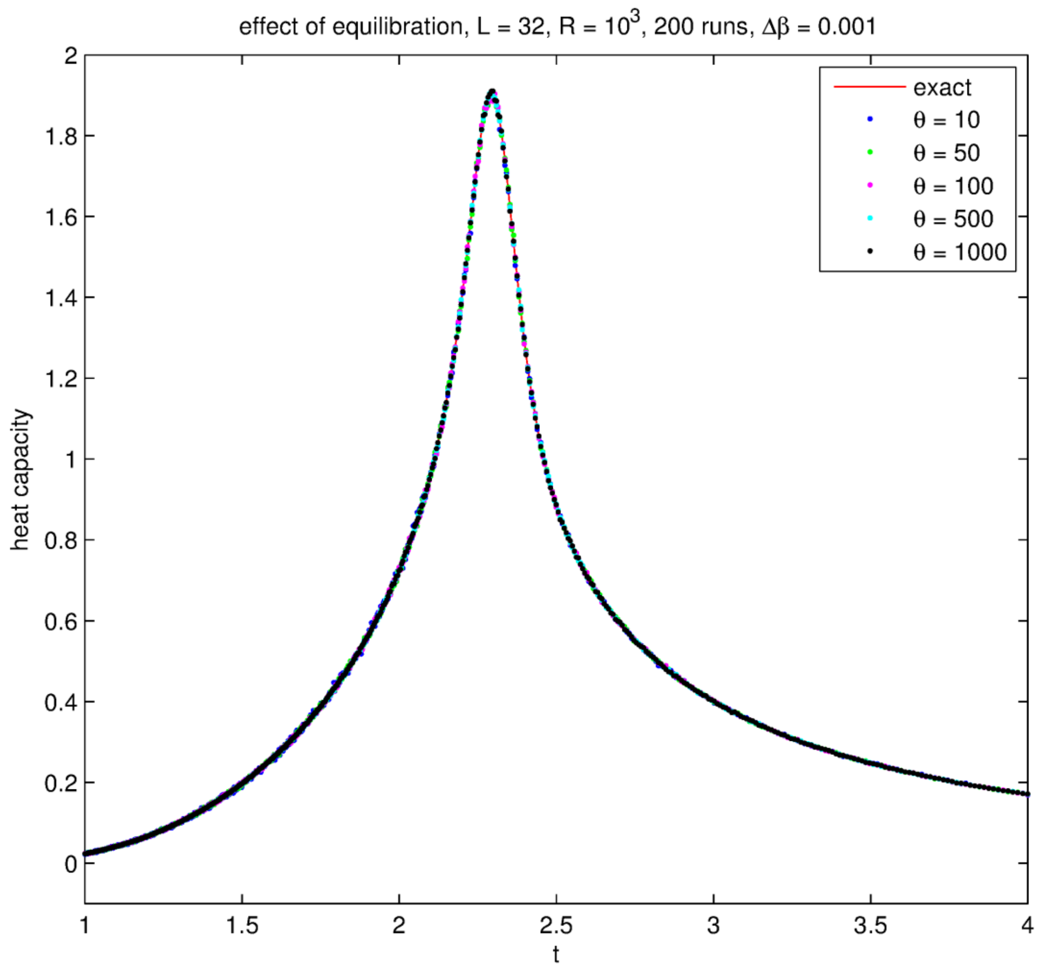


Figure 3: Heat capacity as a function of the temperature for a different number of equilibration sweeps θ.

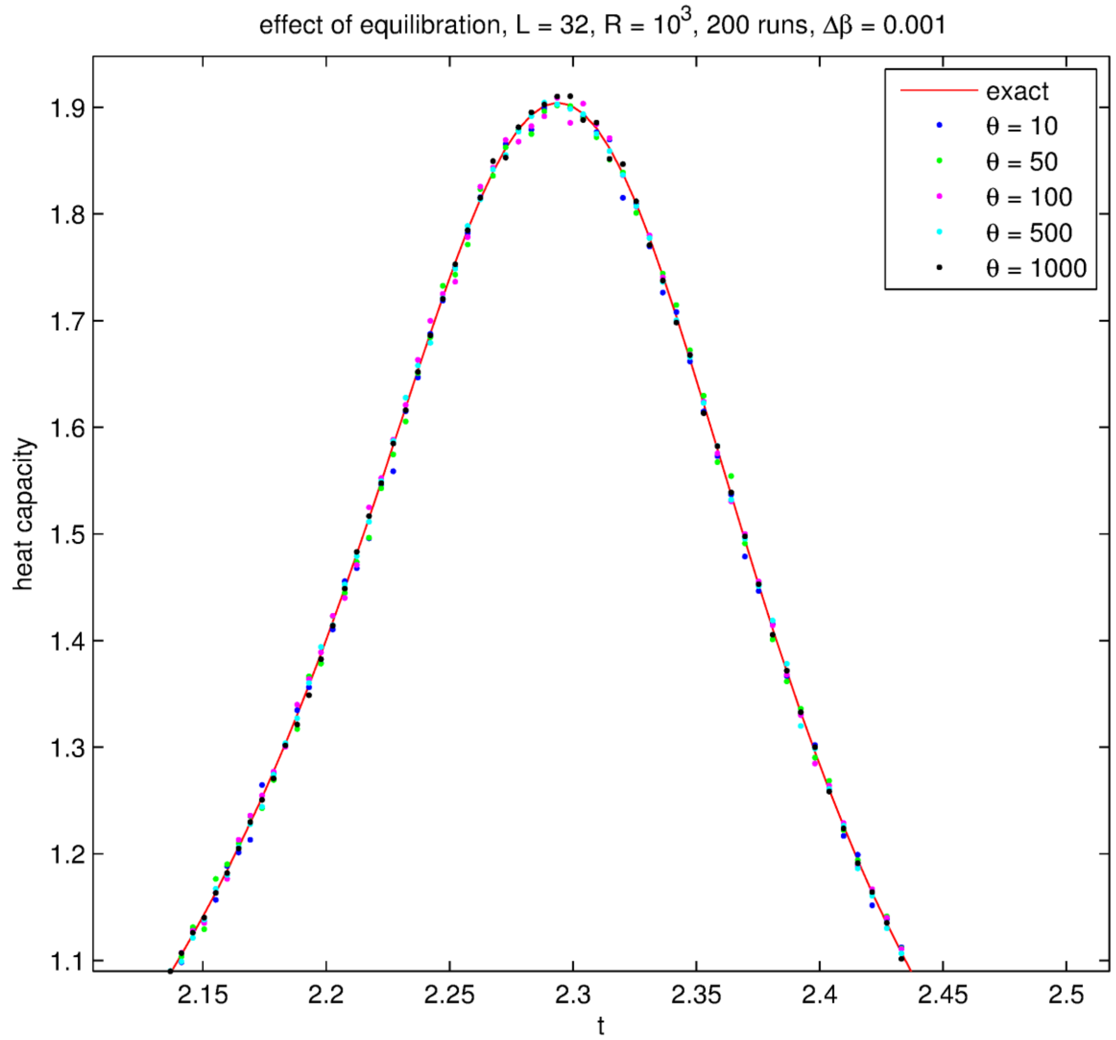


Figure 4: Detail from the previous plot in the critical region.

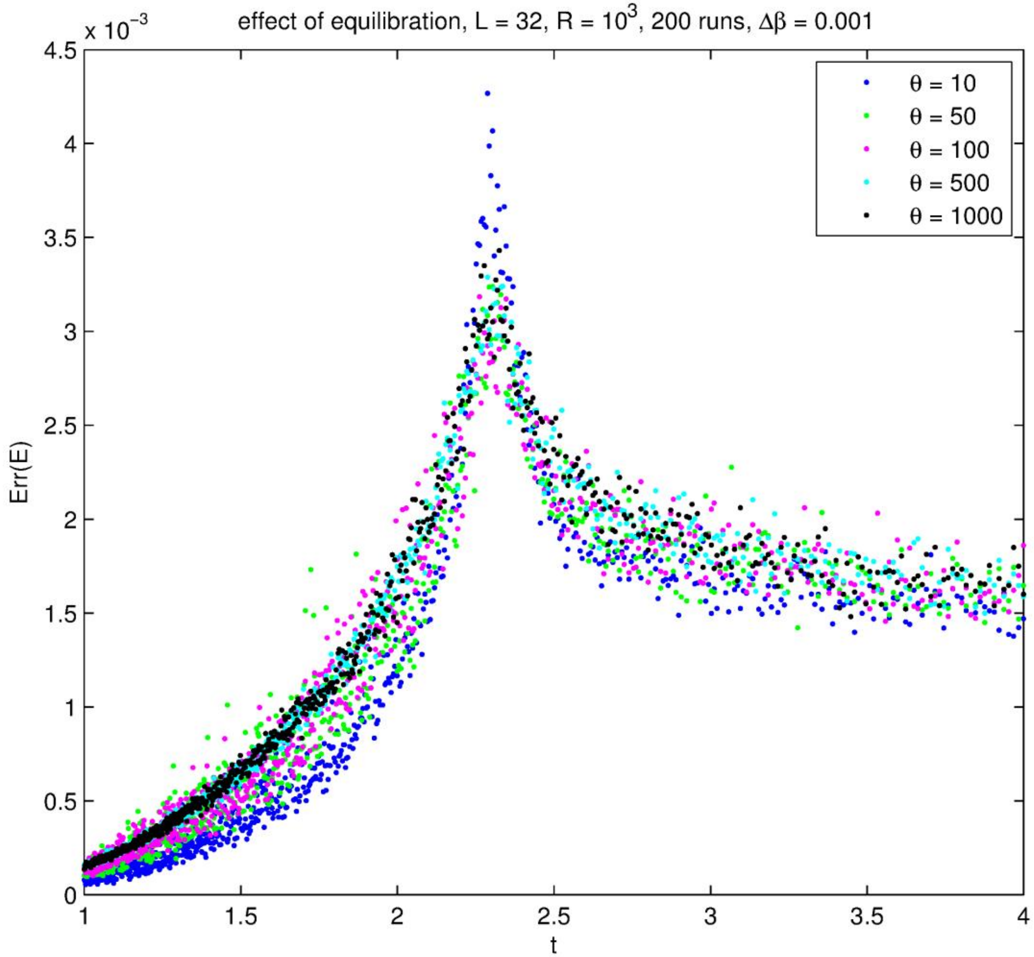


Figure 5: Internal energy error as a function of the temperature for a different number of equilibration sweeps θ.

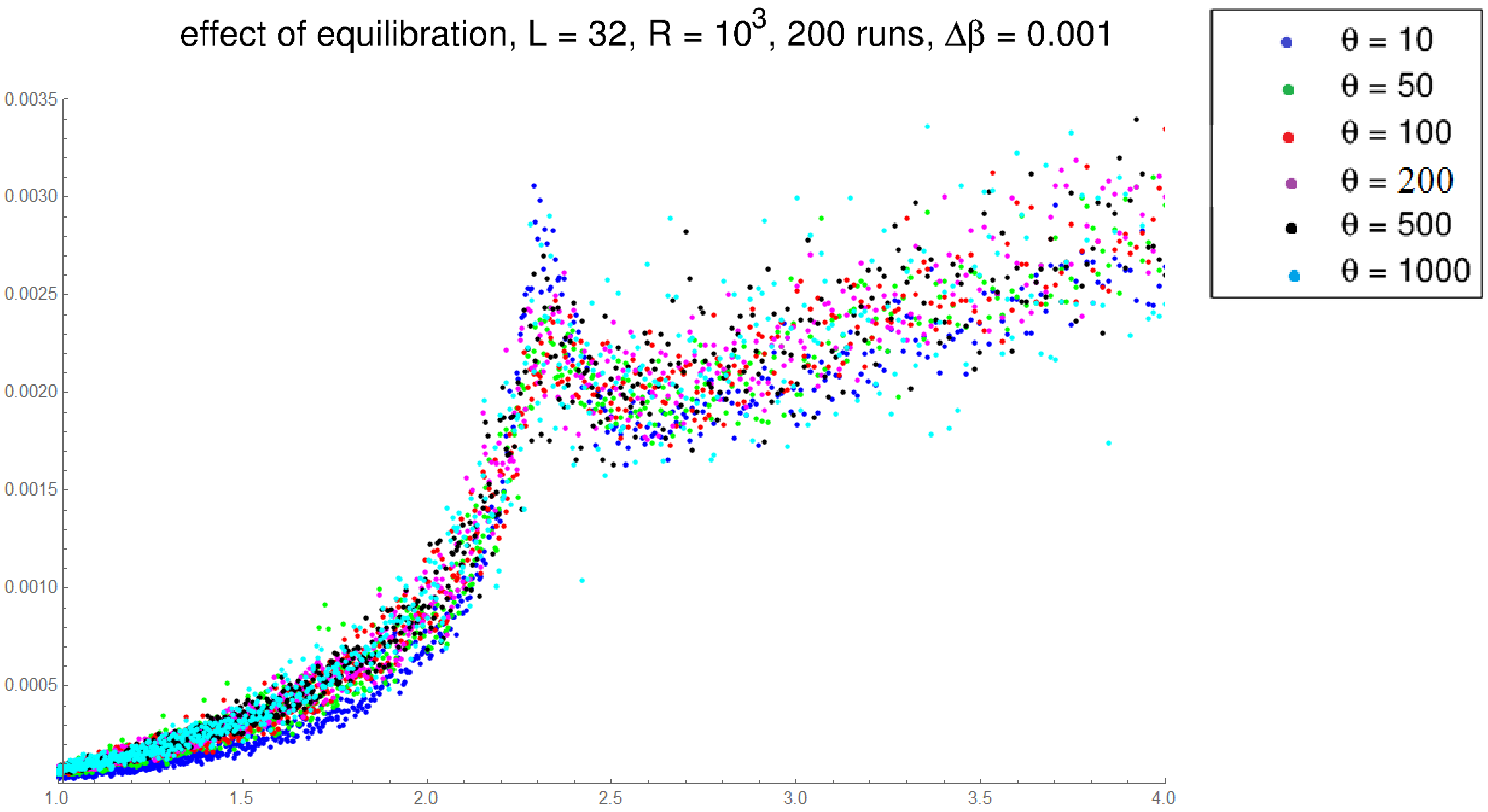


Figure 5a: Internal energy error divided by absolute value of internal energy as a function of the temperature for a different number of equilibration sweeps θ.

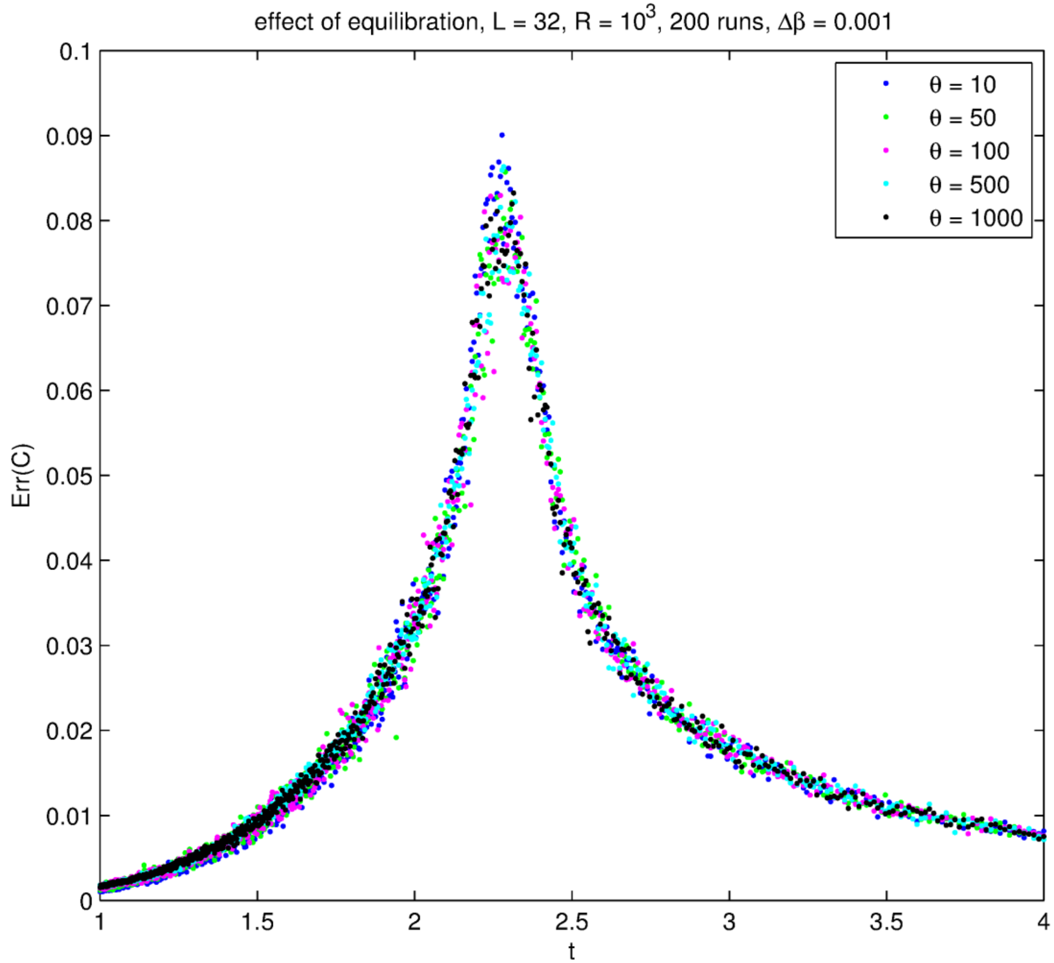


Figure 6: Heat capacity errors as a function of the temperature for a different number of equilibration sweeps θ.

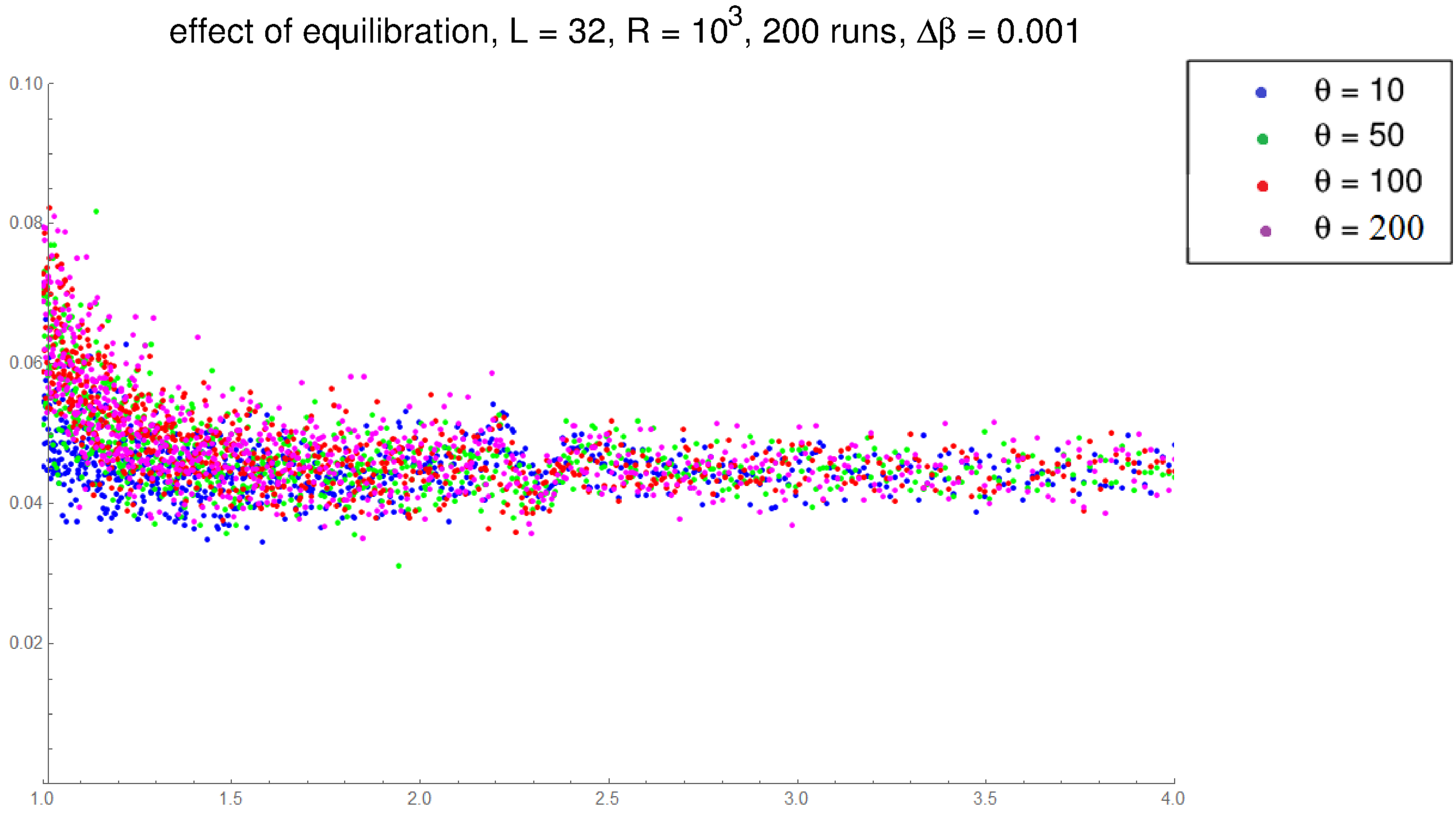


Figure 6a: Heat capacity errors divided by heat capacity as a function of the temperature for a different number of equilibration sweeps θ.

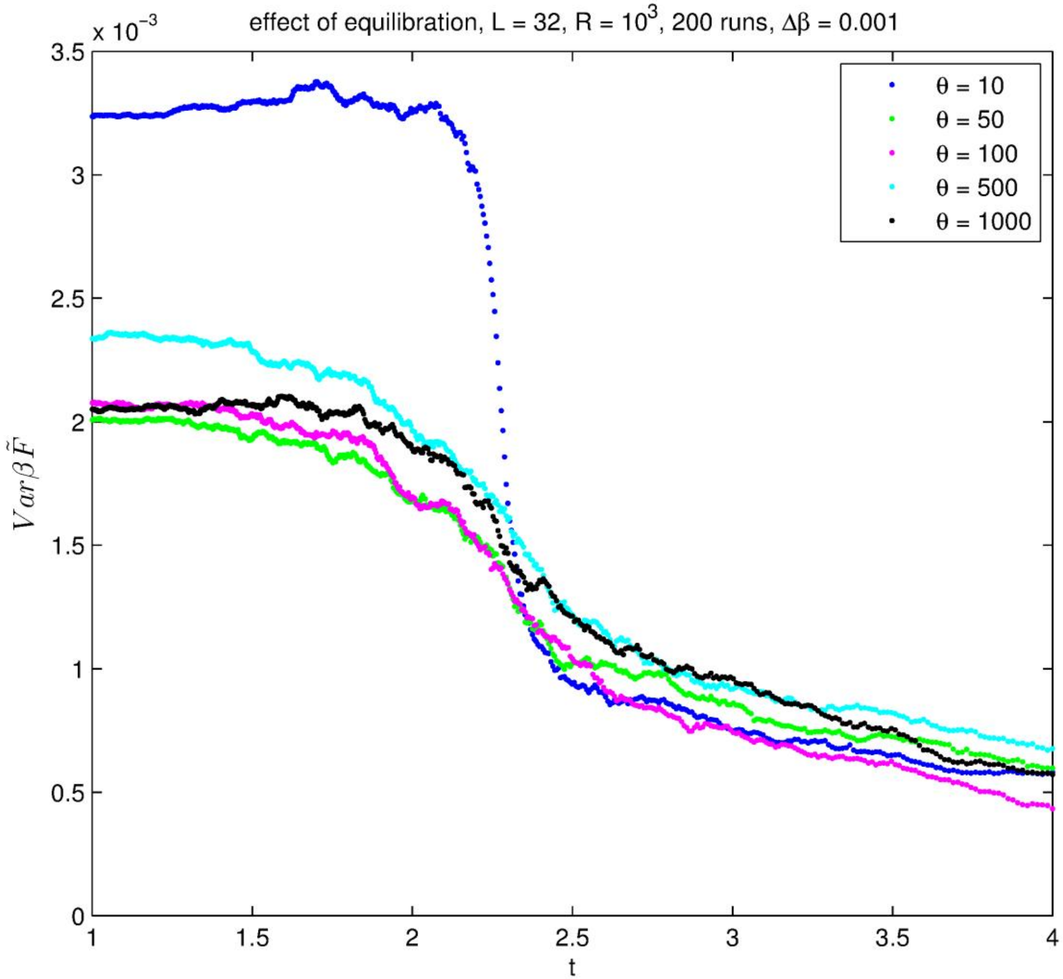


Figure 7: Variance of a dimensionless free energy $\beta\tilde{F}$ as a function of temperature for a different number of equilibration sweeps θ.

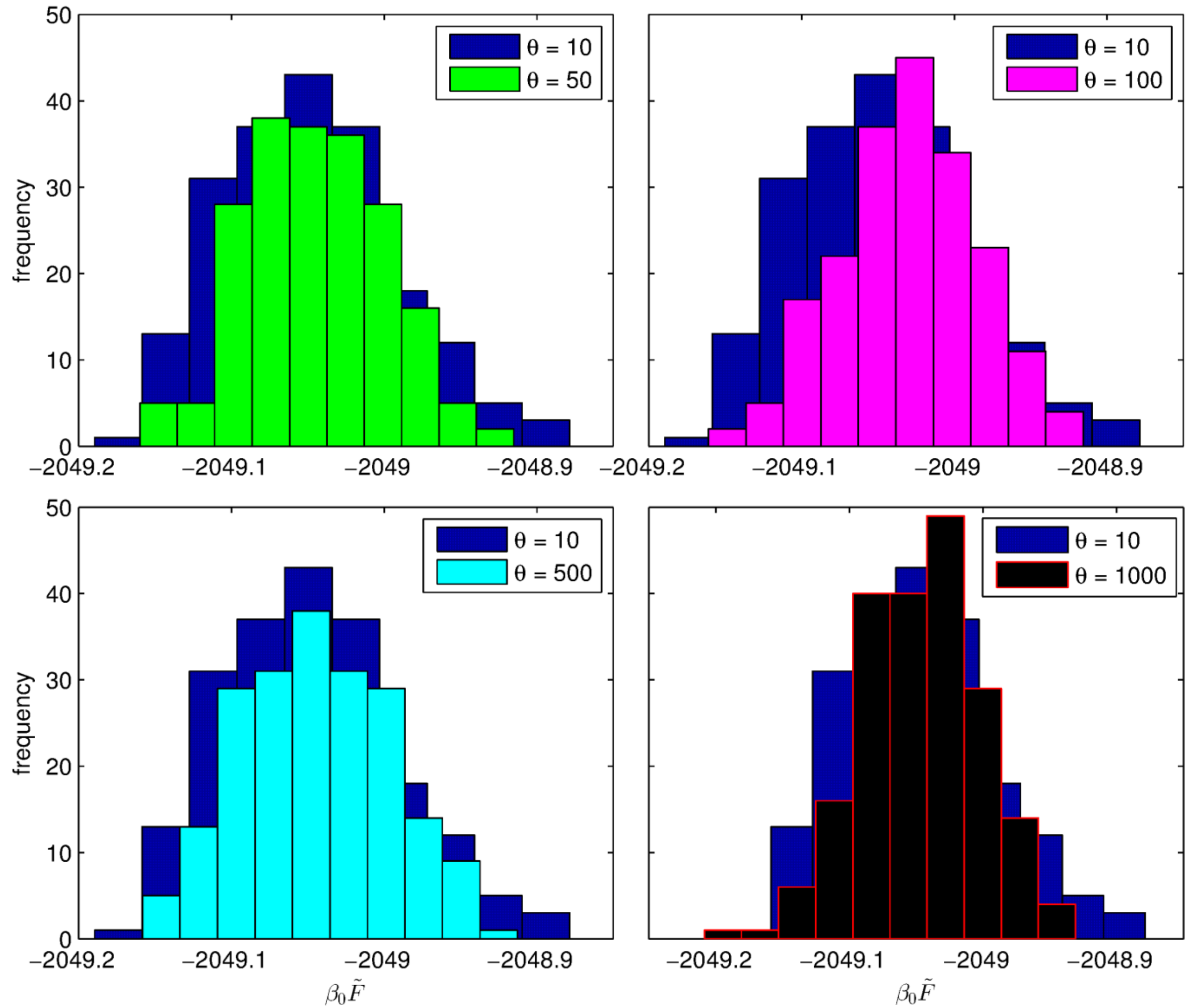


Figure 8: The histograms of a dimensionless free energy $\beta_0 \tilde{F}$ at the temperature $\beta_0 = 1$ for a different number of equilibration sweeps θ. Every subfigure contains the histogram of the non-equilibrated case with $\theta = 10$.

Effect of population size

$\theta = 10^2$, weighted average over $M = 200$ independent runs, $\Delta\beta = 0.001$

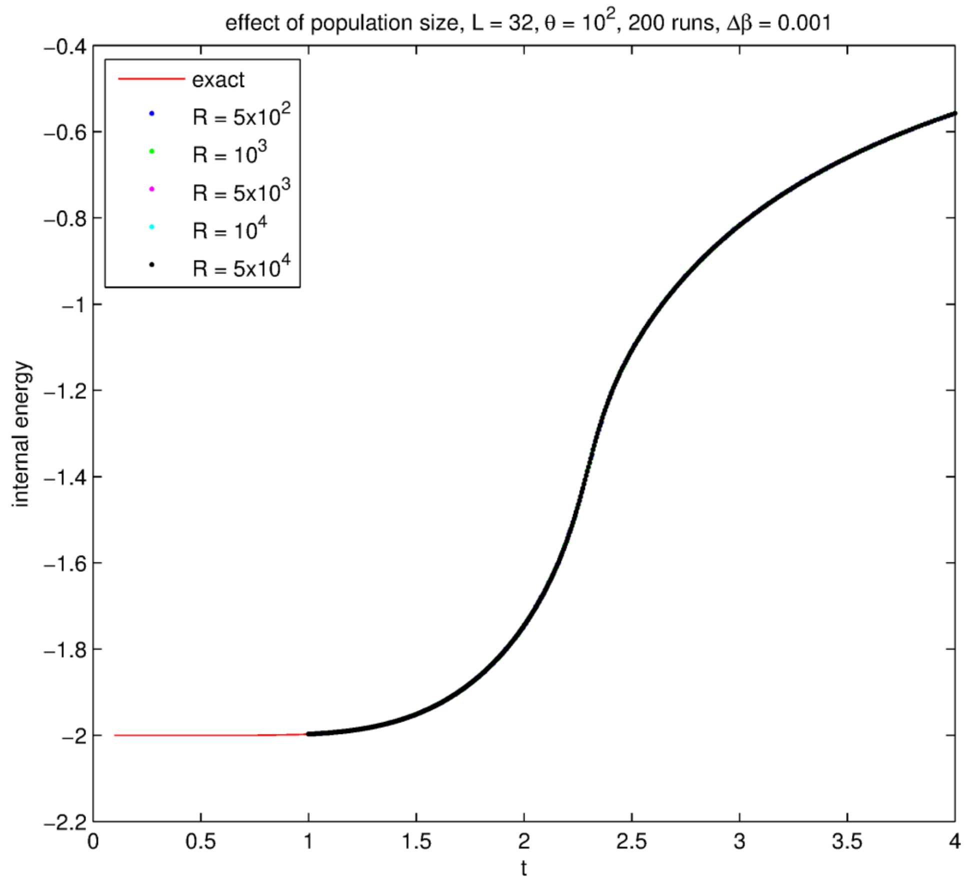


Figure 9: Internal energy per spin as a function of the temperature $t = k_B T/J$ for a different number of replicas R.

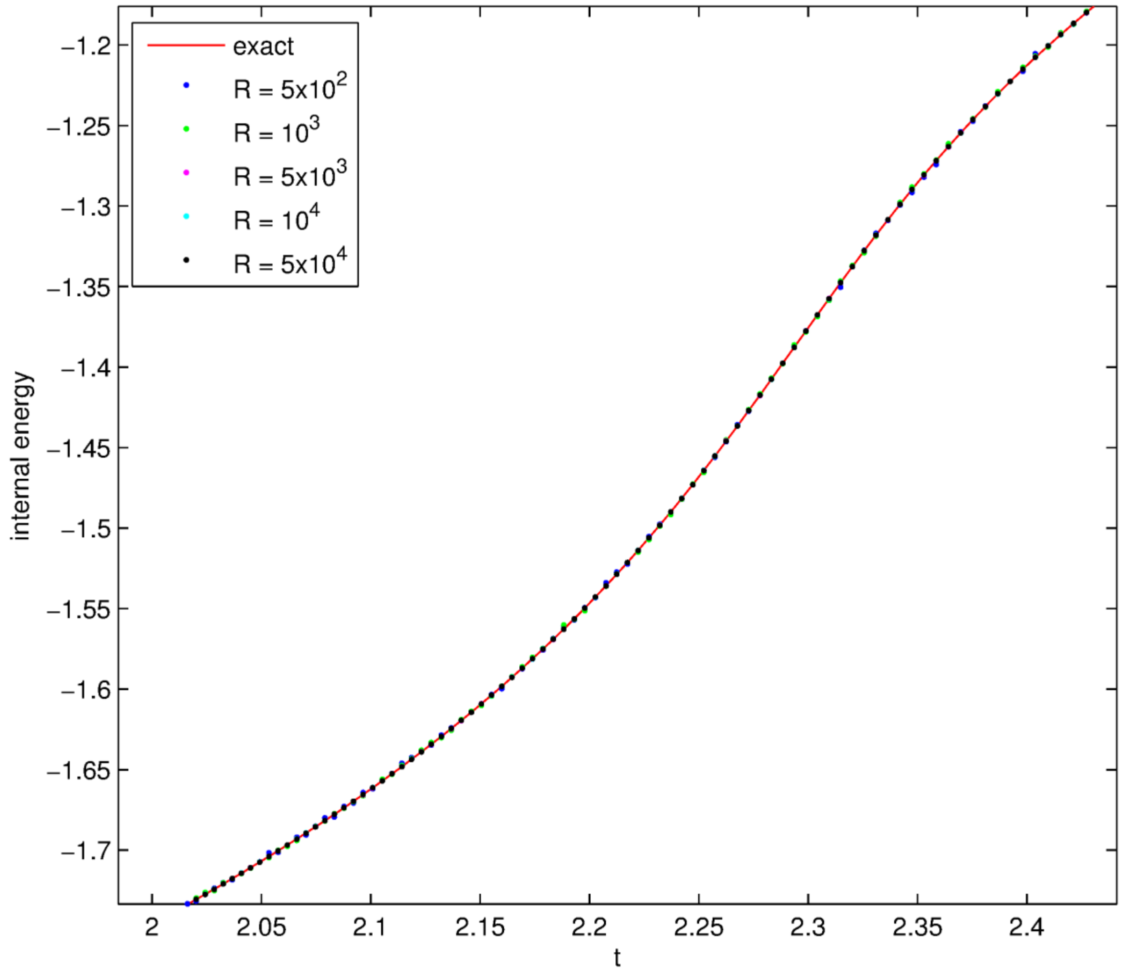


Figure 10: Detail from the previous plot in the critical region.

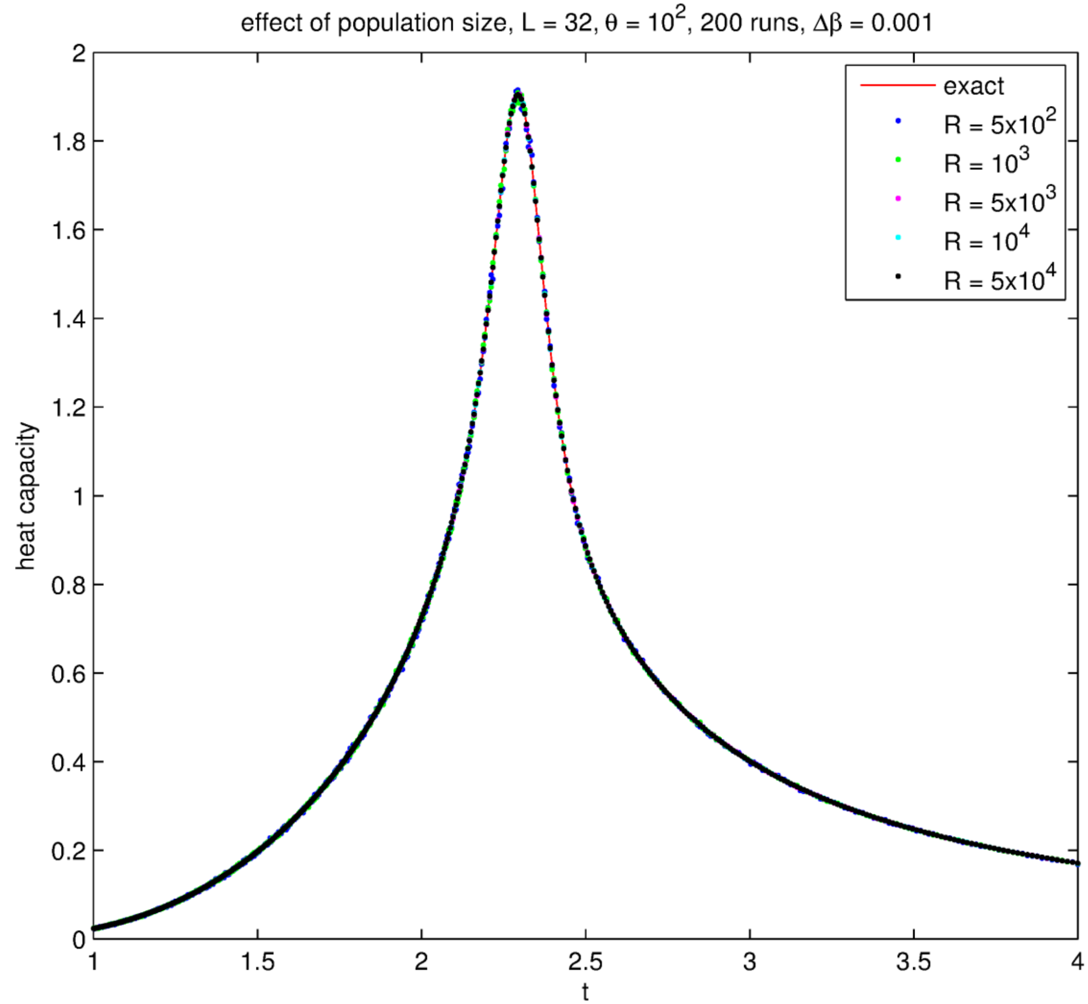


Figure 11: Heat capacity as a function of the temperature for a different number of replicas R.

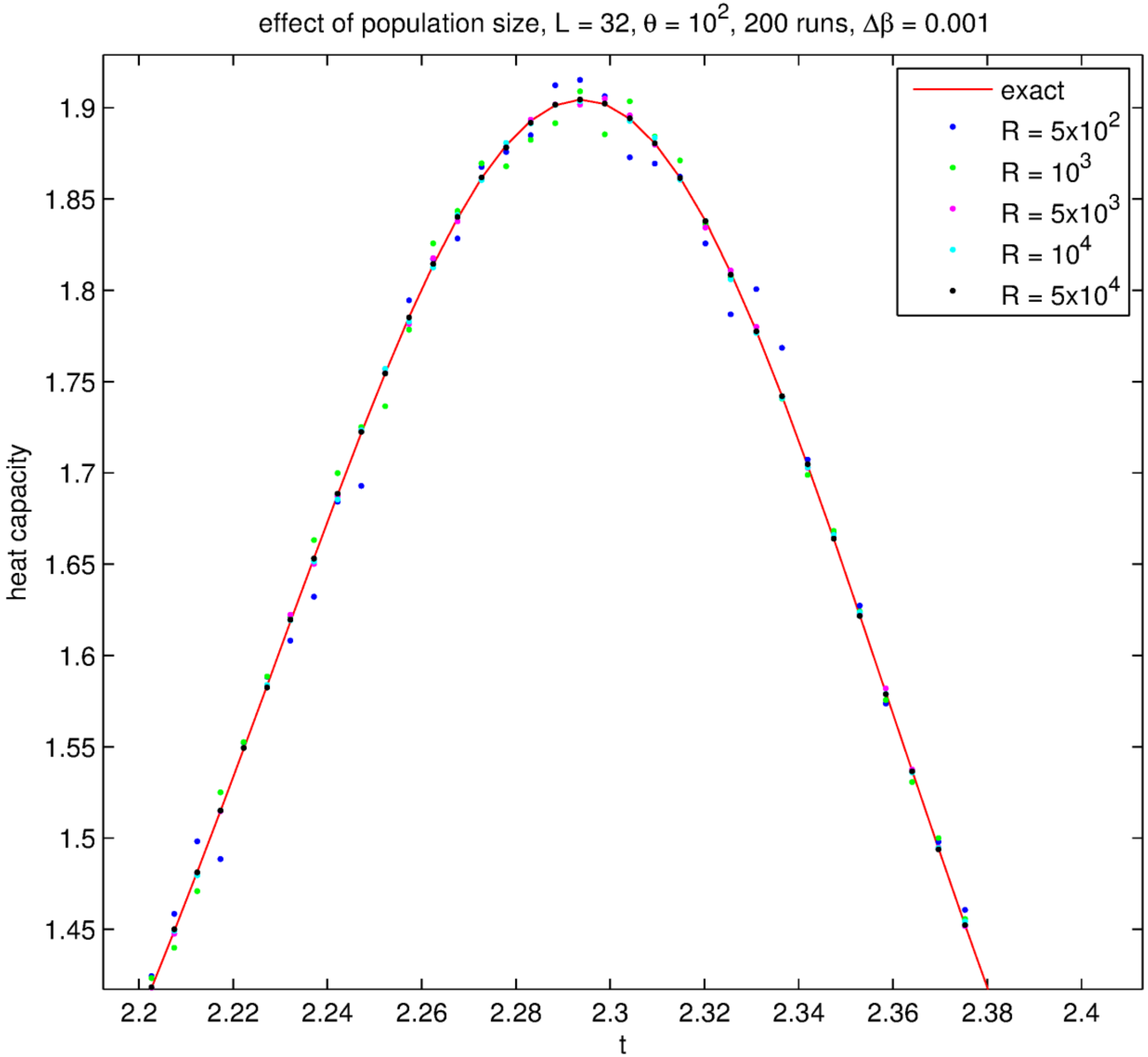


Figure 12: Detail from the previous plot in the critical region.

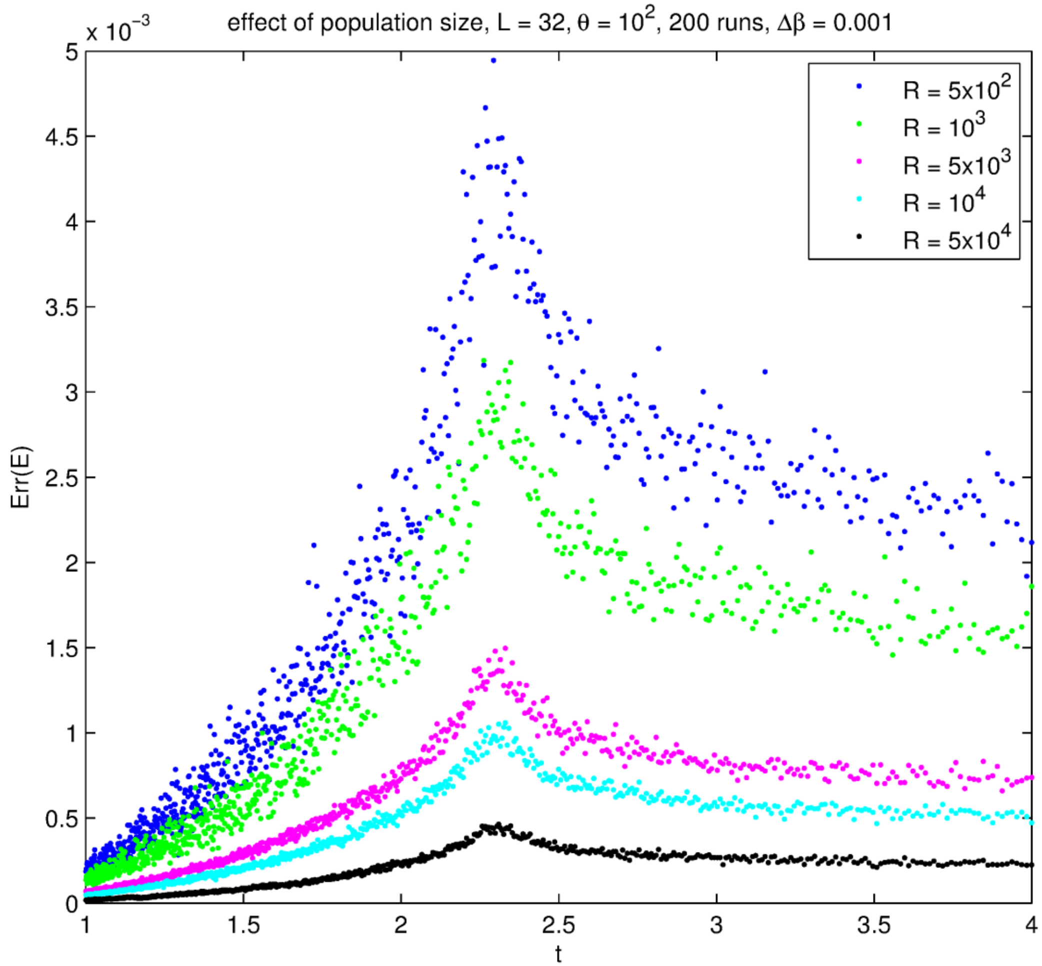


Figure 13: Internal energy error as a function of the temperature for a different number of replicas R.

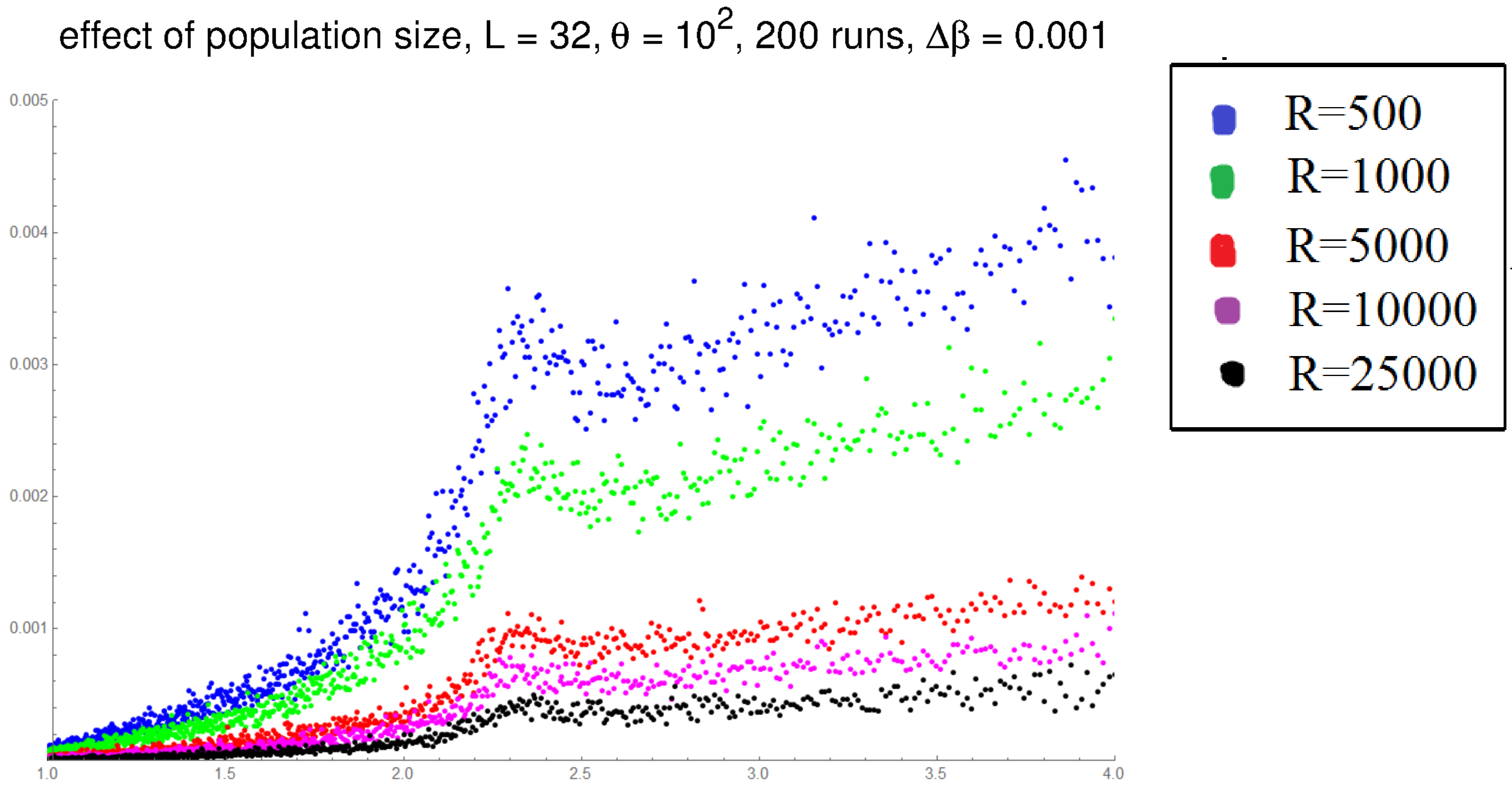


Figure 13a: Internal energy error divided by internal energy as a function of the temperature for a different number of replicas R.

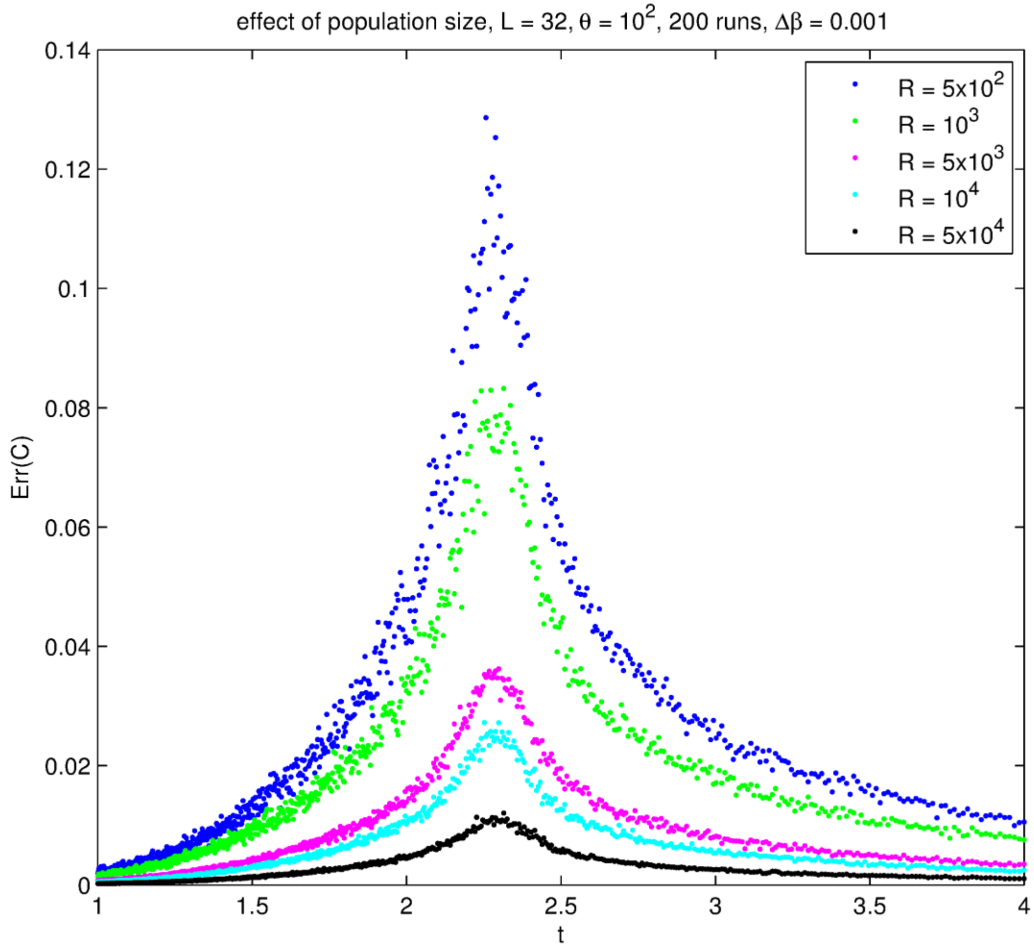


Figure 14: Heat capacity errors as a function of the temperature for a different number of replicas R.

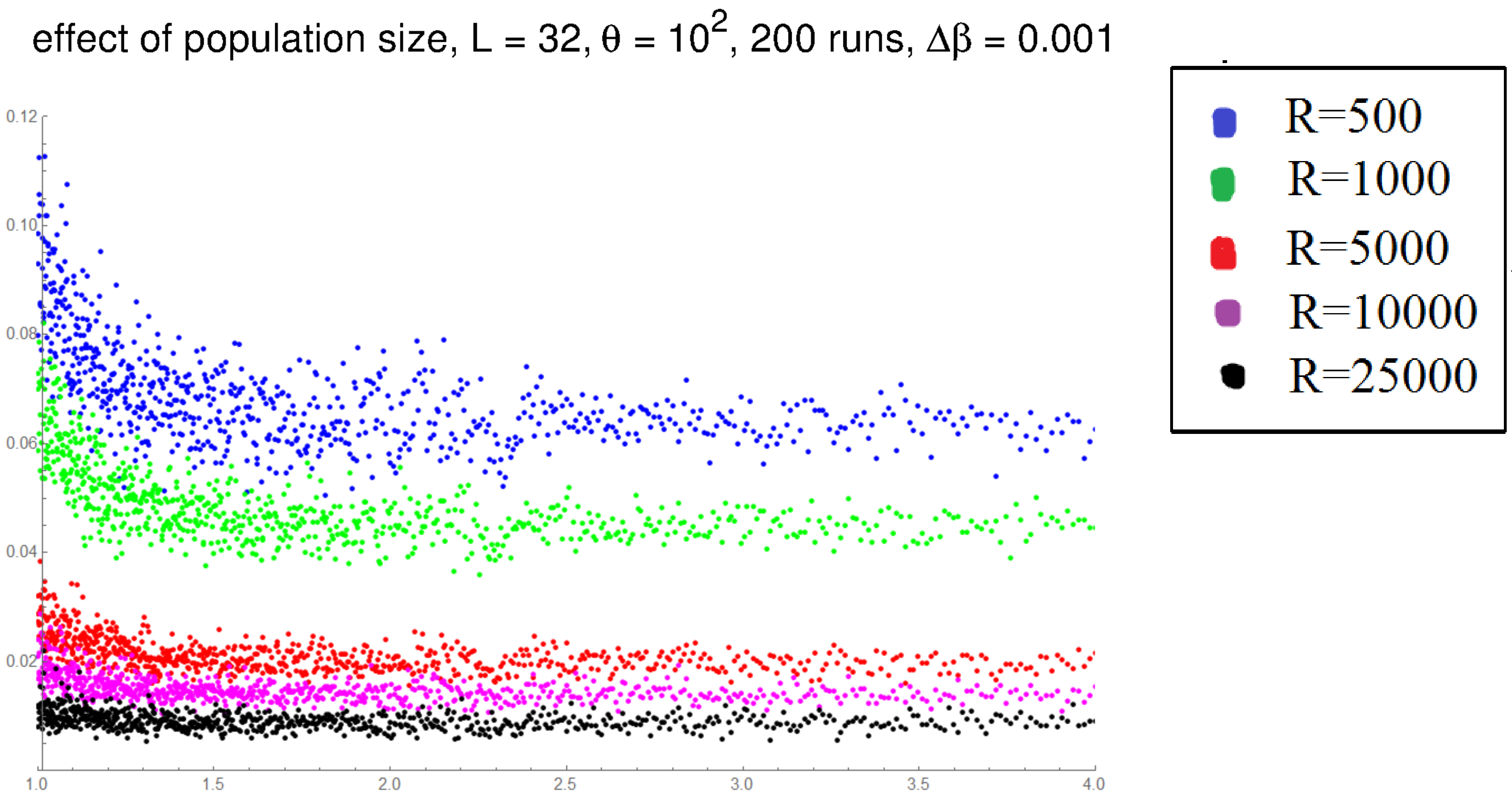


Figure 14a: Heat capacity errors divided by heat capacity as a function of the temperature for a different number of replicas R.

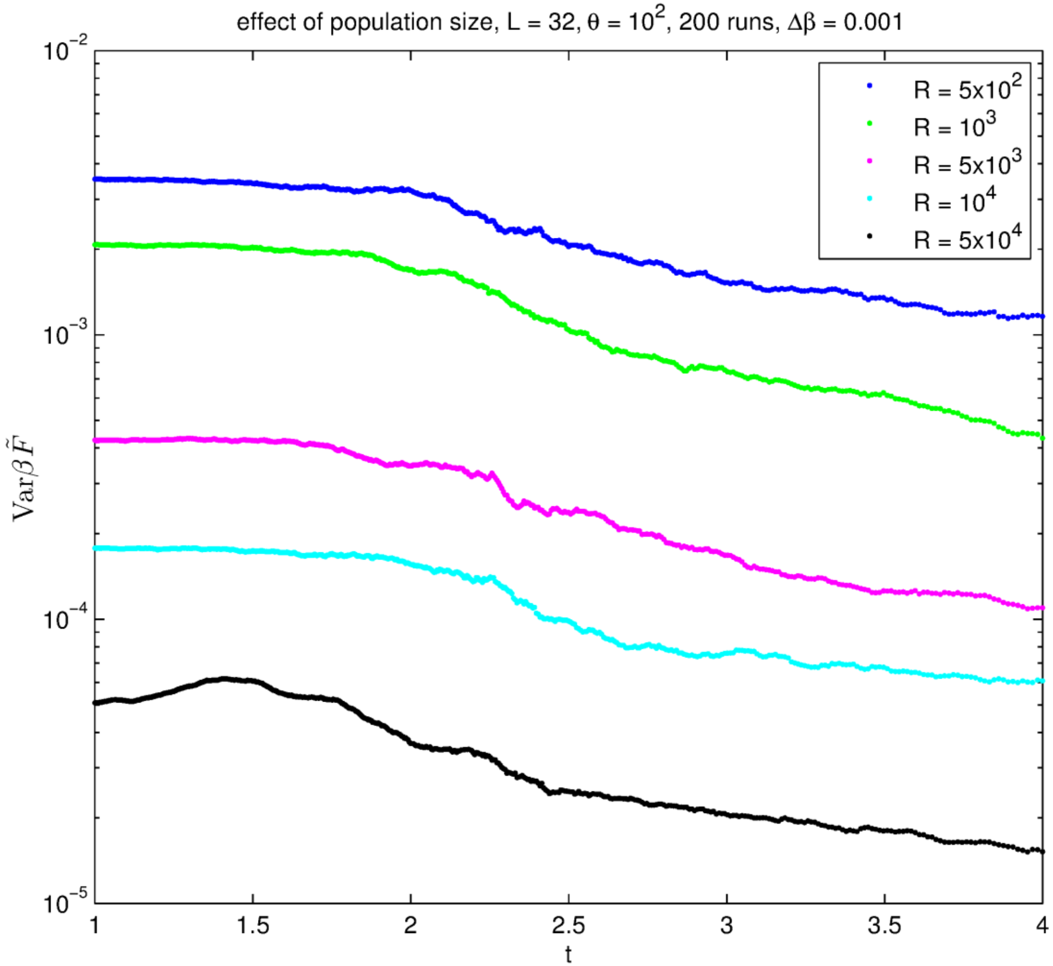


Figure 15: Variance of a dimensionless free energy $\beta\tilde{F}$ as a function of temperature for a different number of replicas R.

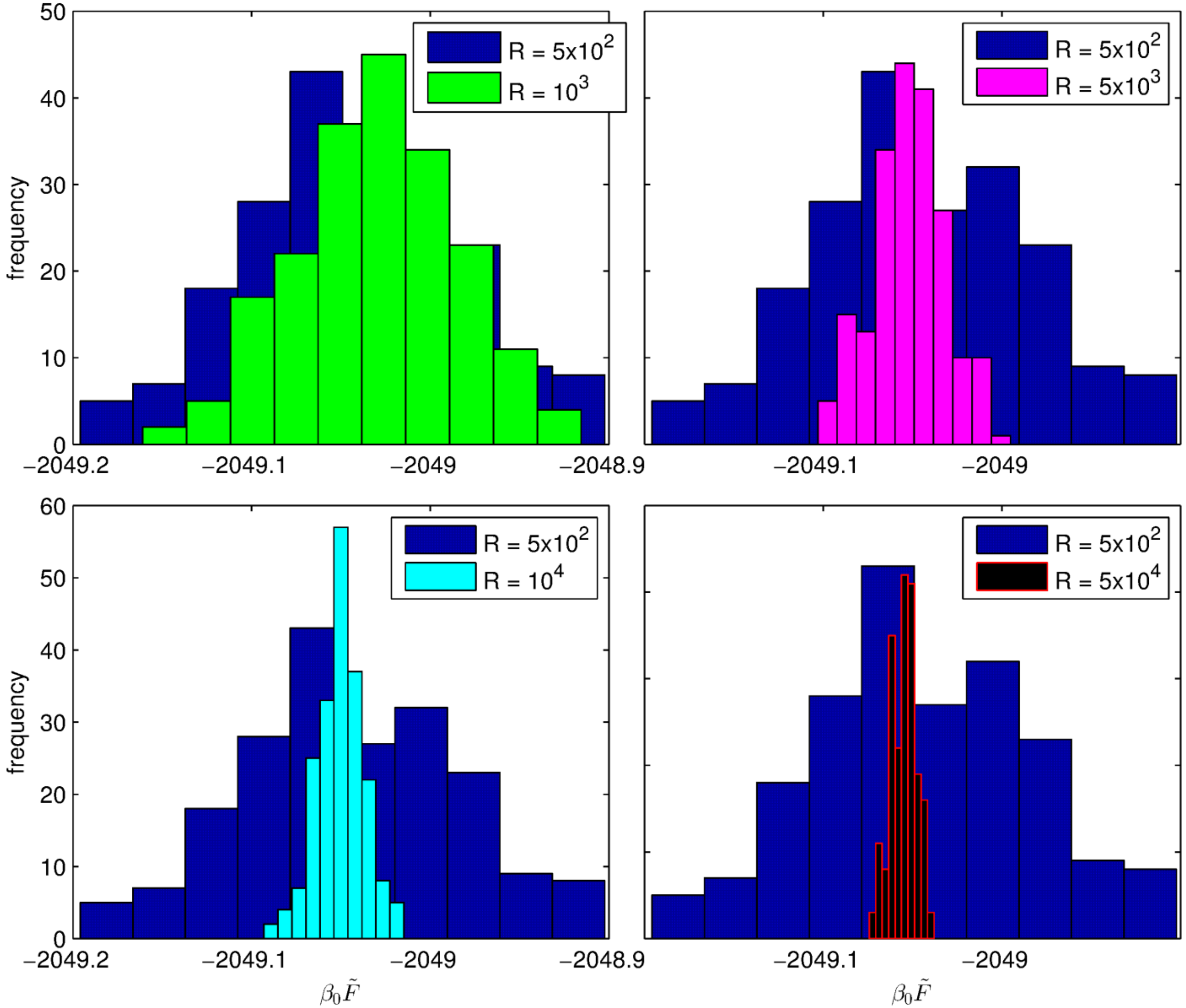


Figure 16: The histograms of a dimensionless free energy $\beta_0\tilde{F}$ at the temperature $\beta_0 = 1$ for a different number of replicas R.

Weighted average over ensemble of independent runs
$R = 10^3$, $\theta = 10^3$, $\Delta\beta = 0.001$

Unbiased estimate of observable $\tilde{A}$ from M independent runs:

$$\bar{A}(\beta) = \sum_{r=1}^{M} \tilde{A}_r(\beta)\omega_r(\beta), \tag{1}$$

where the weight of a run r is given by

$$\omega_r(\beta) = \frac{e^{-\beta \tilde{F}_r(\beta)}}{\sum\limits_{r=1}^{M} e^{-\beta \tilde{F}_r(\beta)}}. \tag{2}$$

Errors in weighted averages can be obtained by resampling. In our case, we use bootstraps method, which is defined as follows

$$\sigma_A(\beta) = \sqrt{\mathrm{Var}\,(A(\beta))}, \tag{3}$$

where

$$\mathrm{Var}\,(A(\beta)) = \left\langle \left(\tilde{A}(\beta) - \bar{A}(\beta)\right)^2 \right\rangle. \tag{4}$$

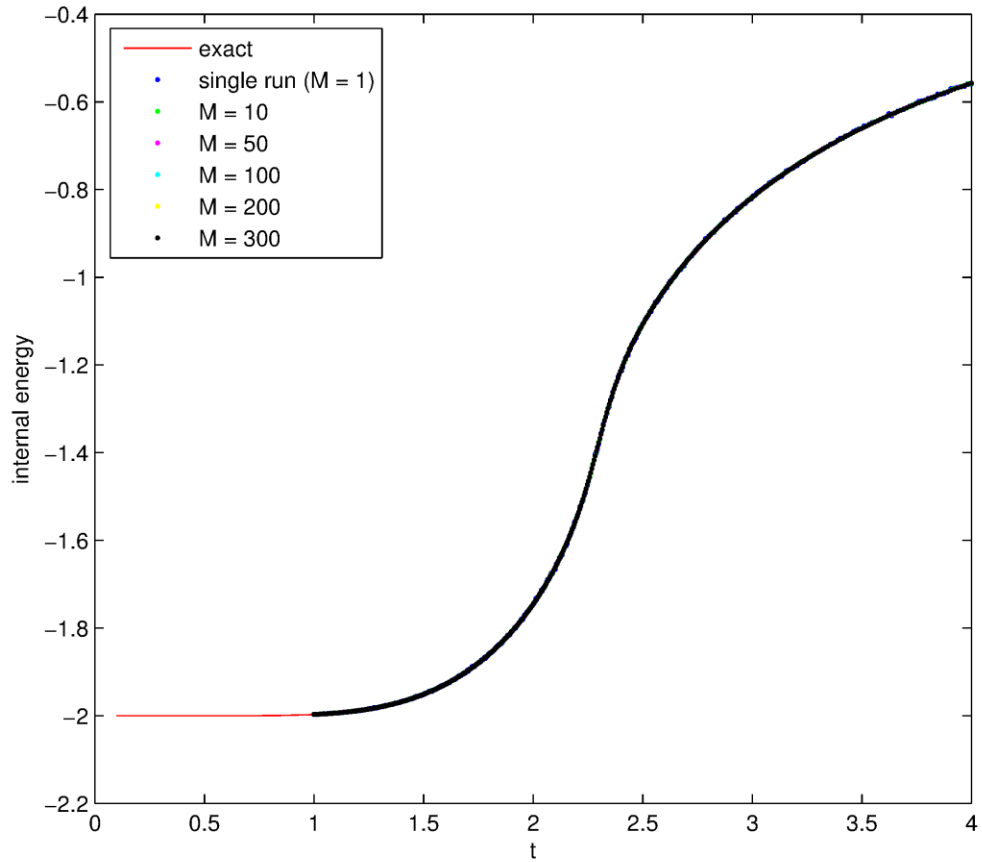


Figure 17: Internal energy per spin as a function of the temperature $t = k_B T/J$ for a different number of independent runs M.

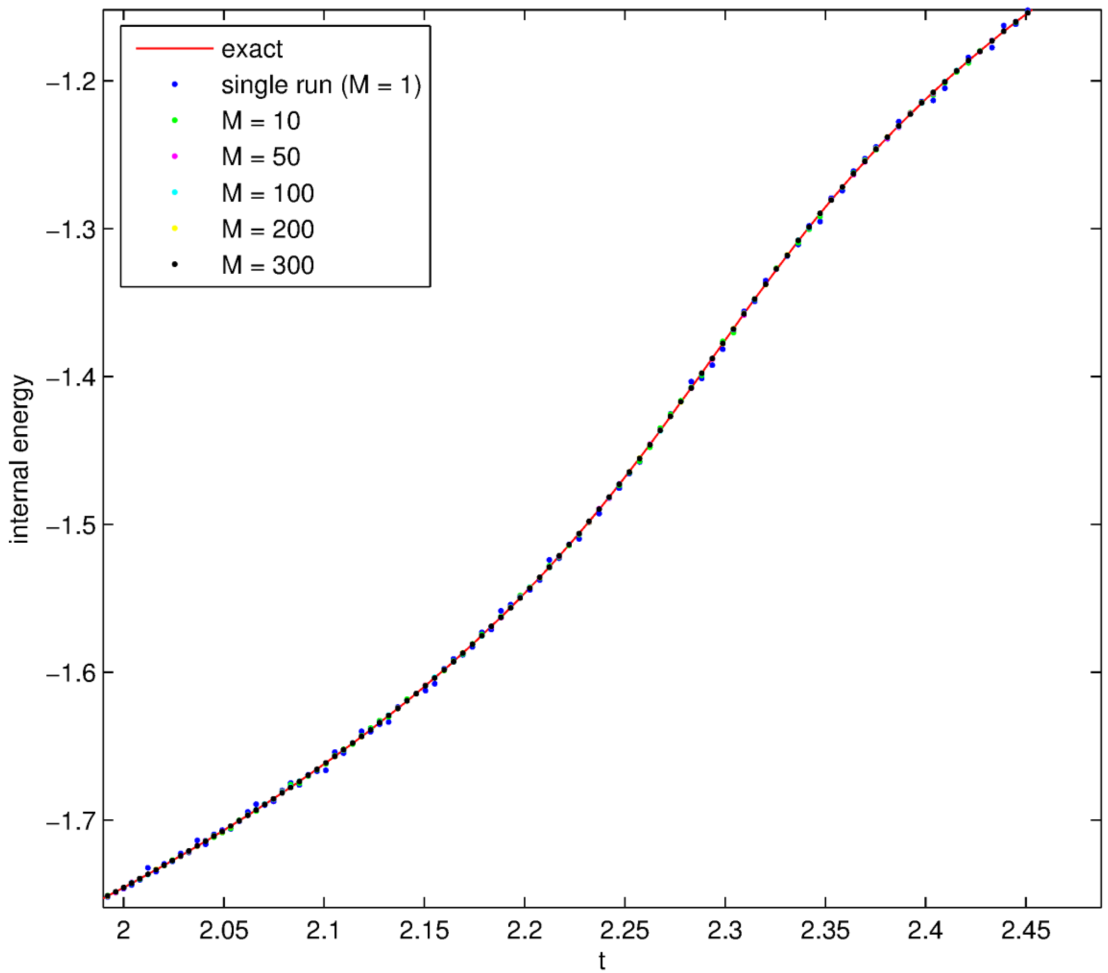


Figure 18: Detail from the previous plot in the critical region.

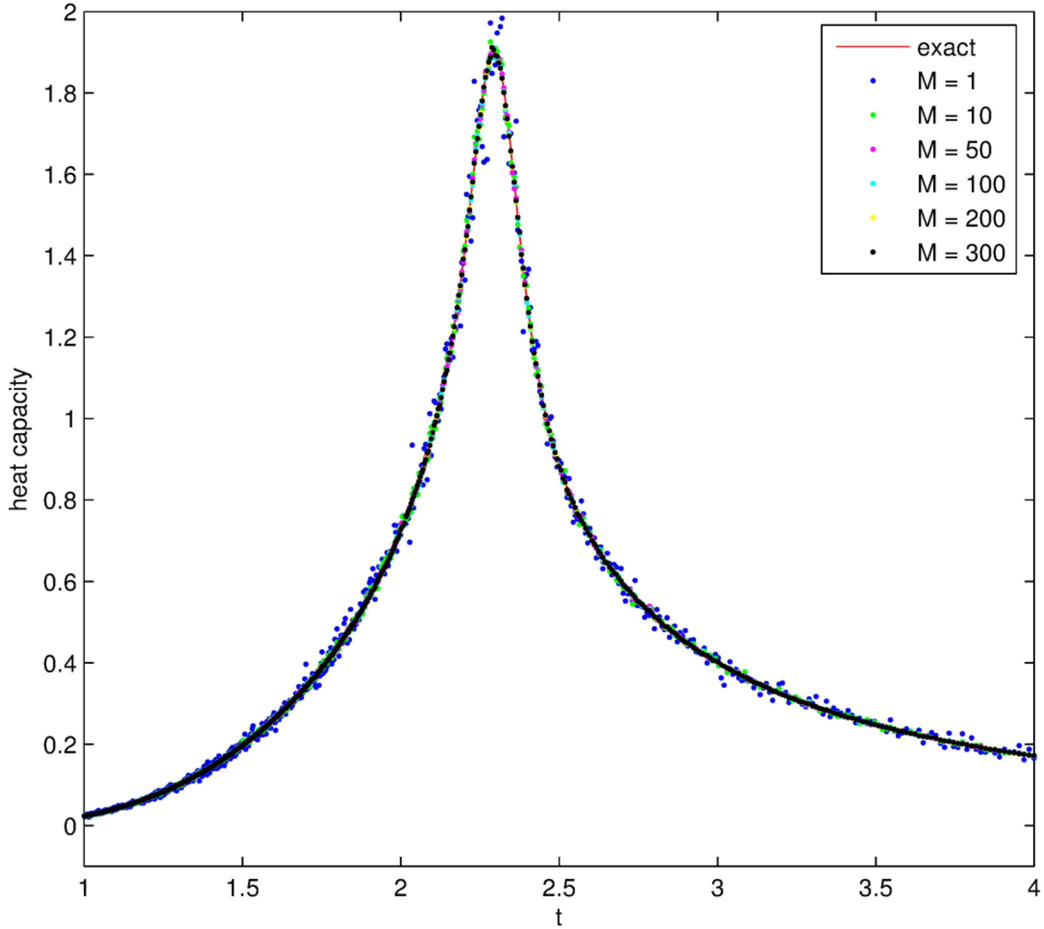


Figure 19: Heat capacity as a function of the temperature for a different number of independent runs M.

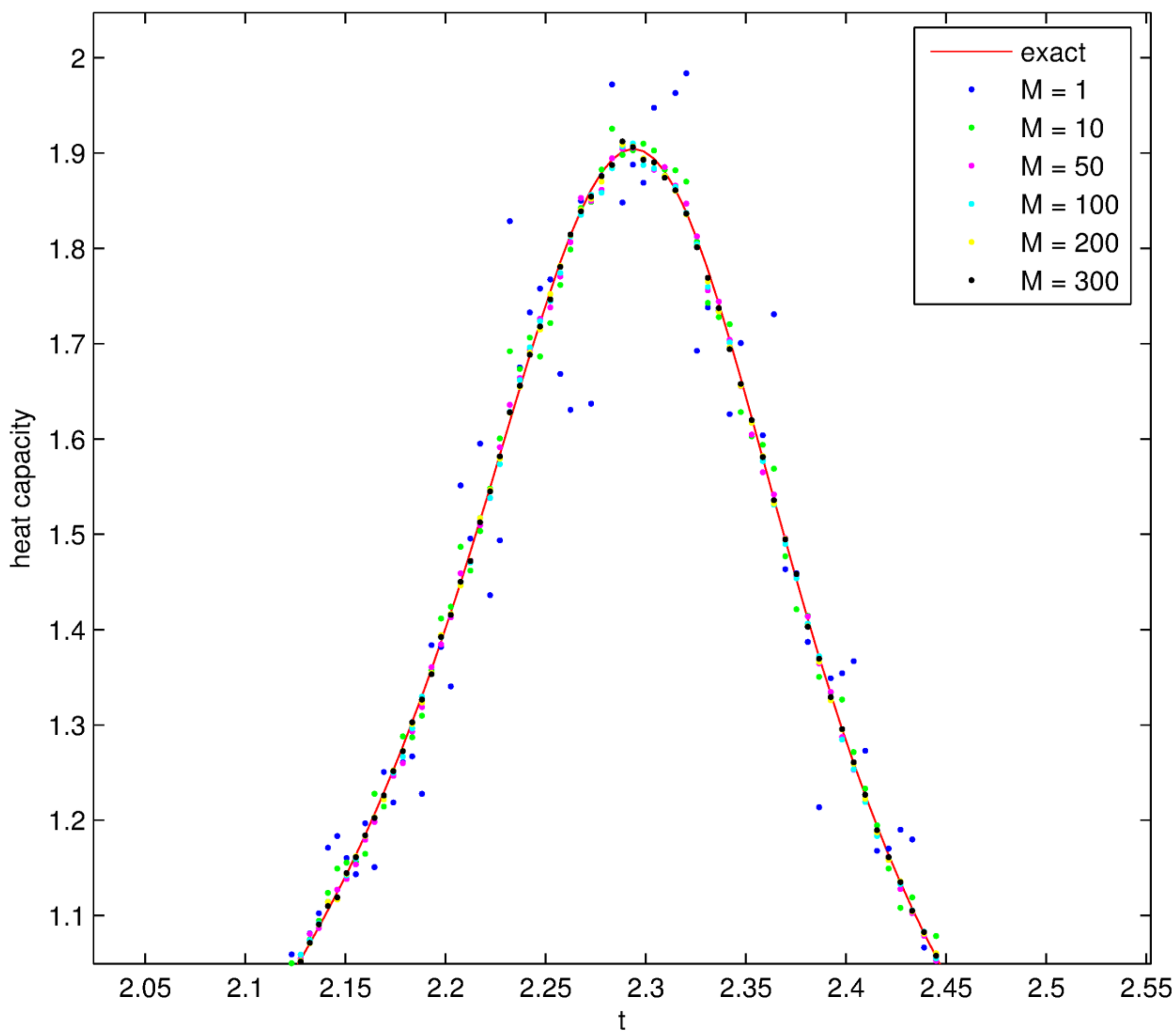
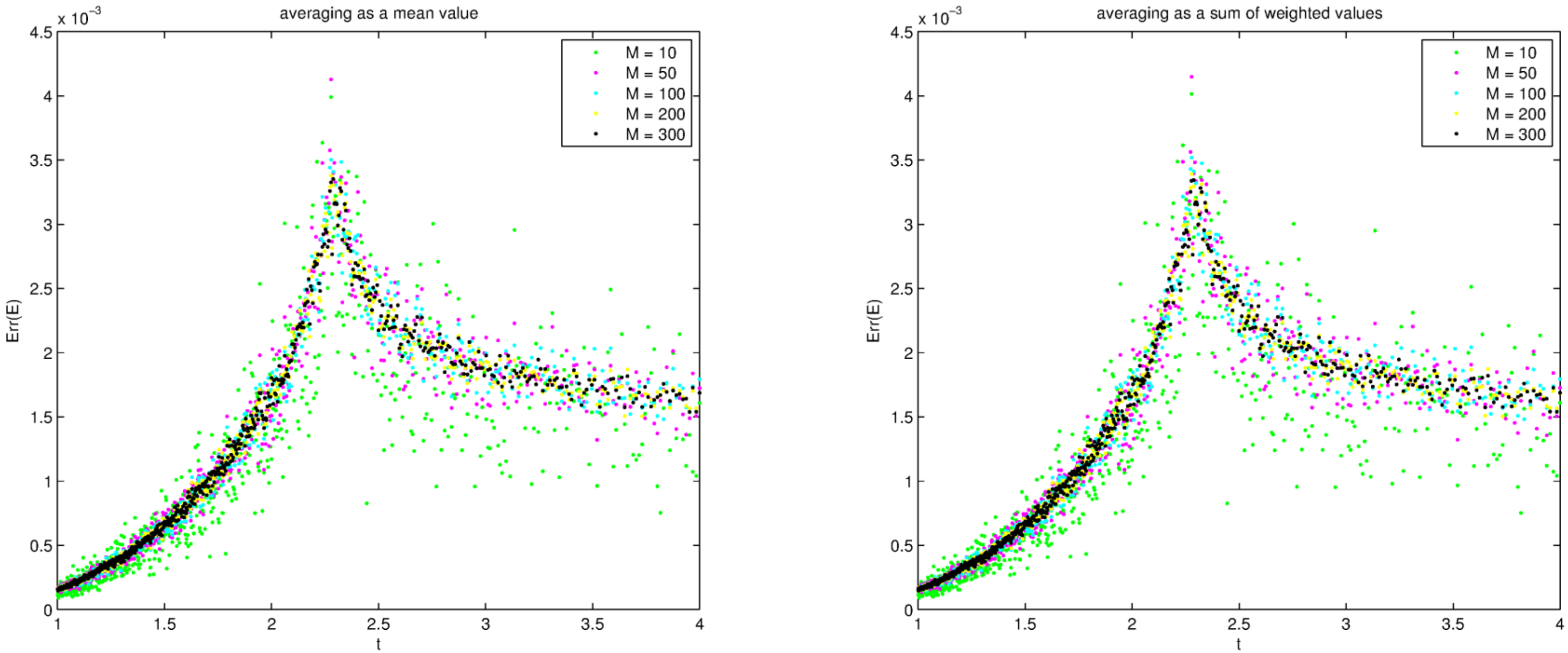


Figure 20: Detail from the previous plot in the critical region.



(a) (b)

Figure 21: Internal energy error as a function of the temperature for a different number of independent runs M.

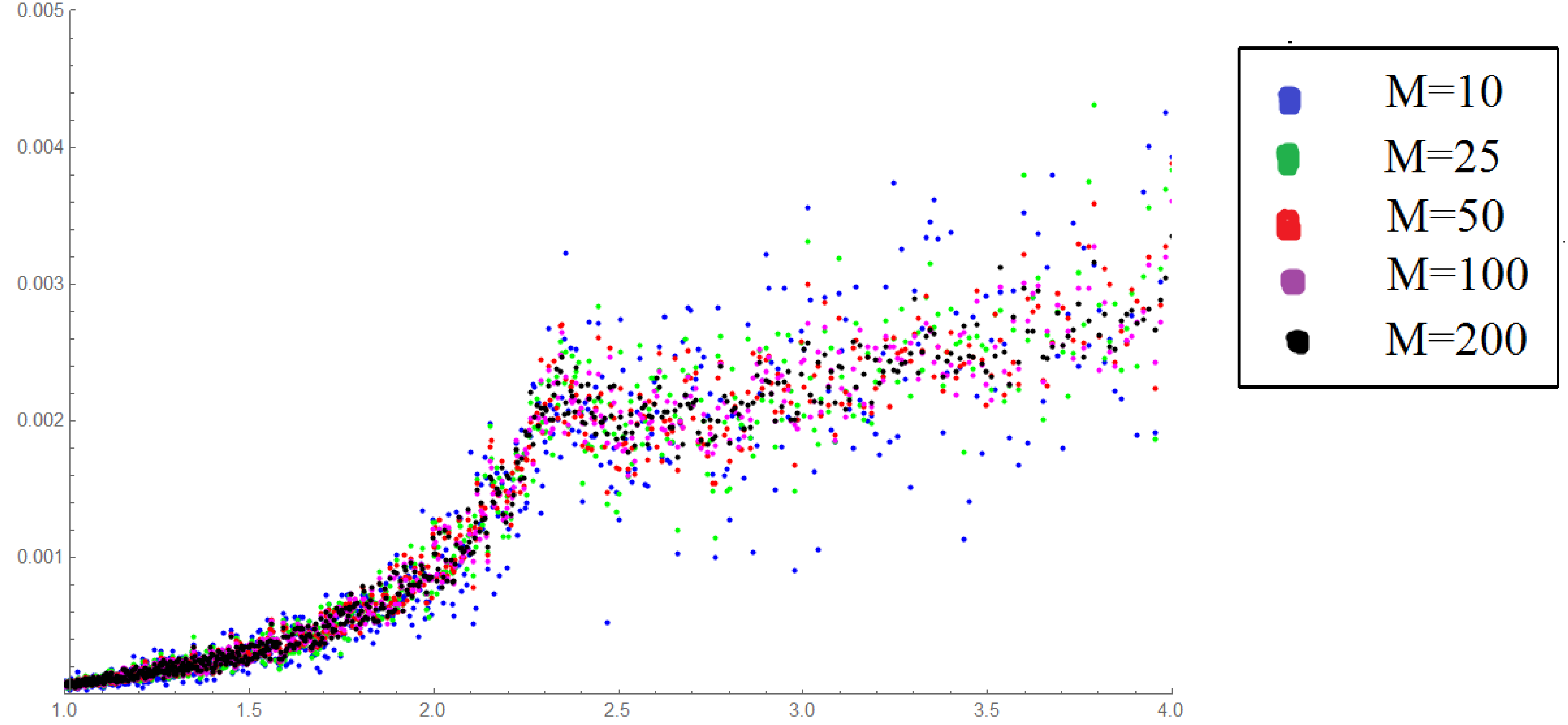
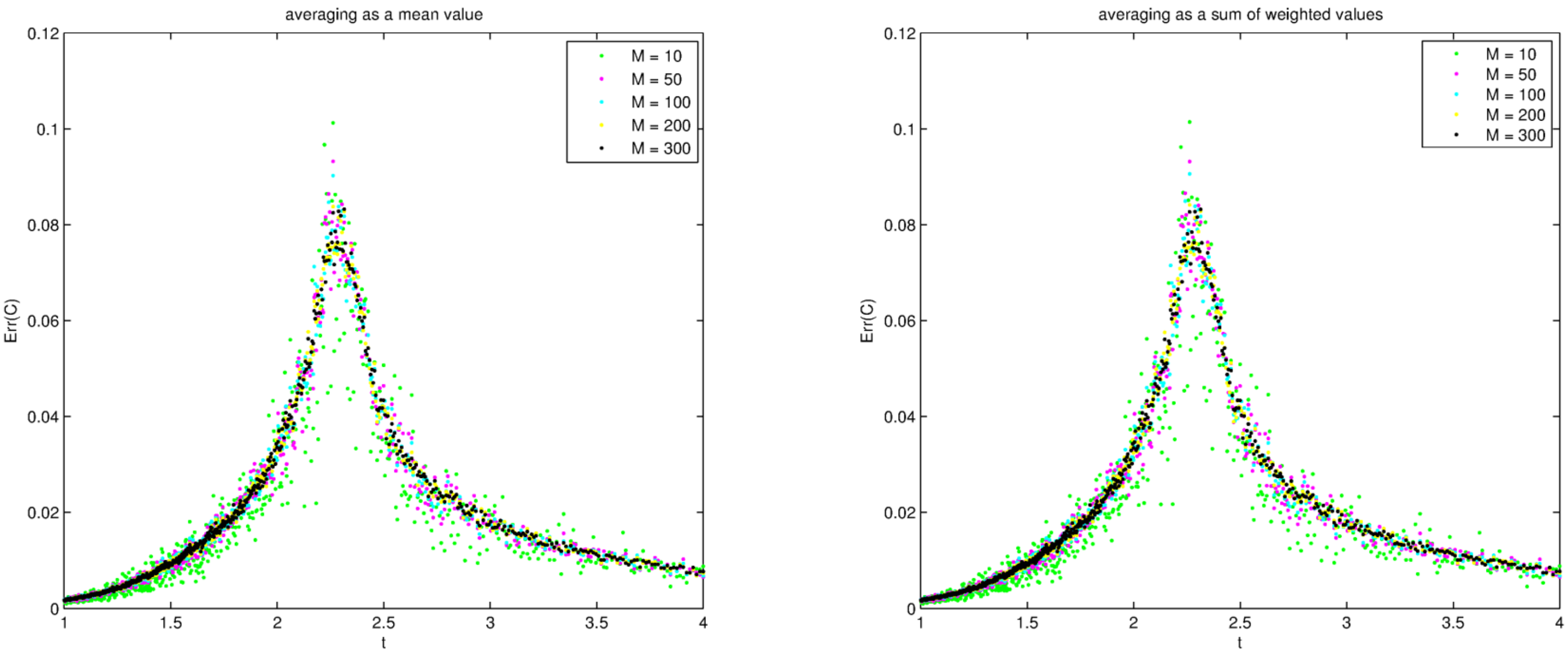


Figure 21a: Internal energy error divided by internal energy as a function of the temperature for a different number of independent runs M.



(a) (b)

Figure 22: Heat capacity errors as a function of the temperature for a different number of independent runs M.

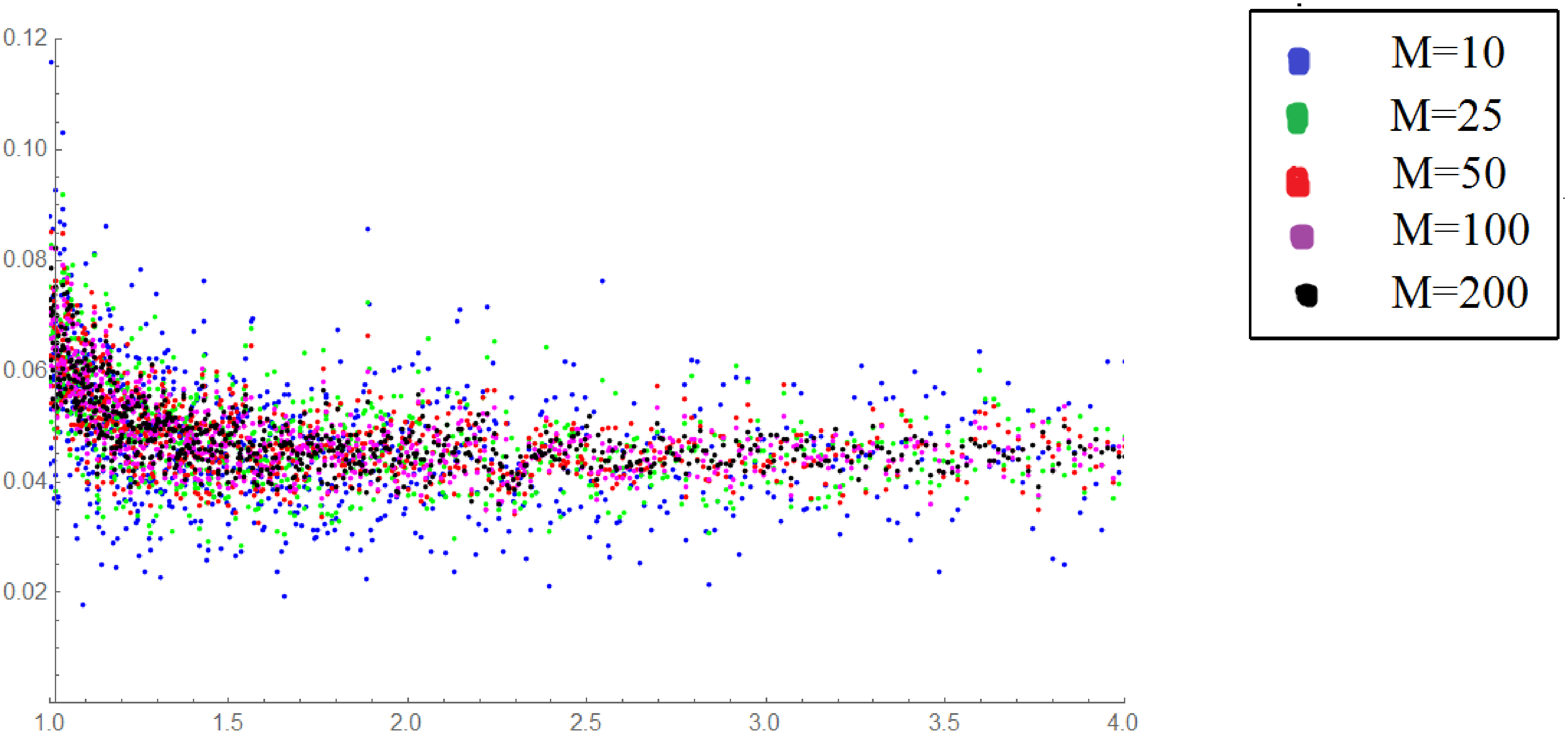
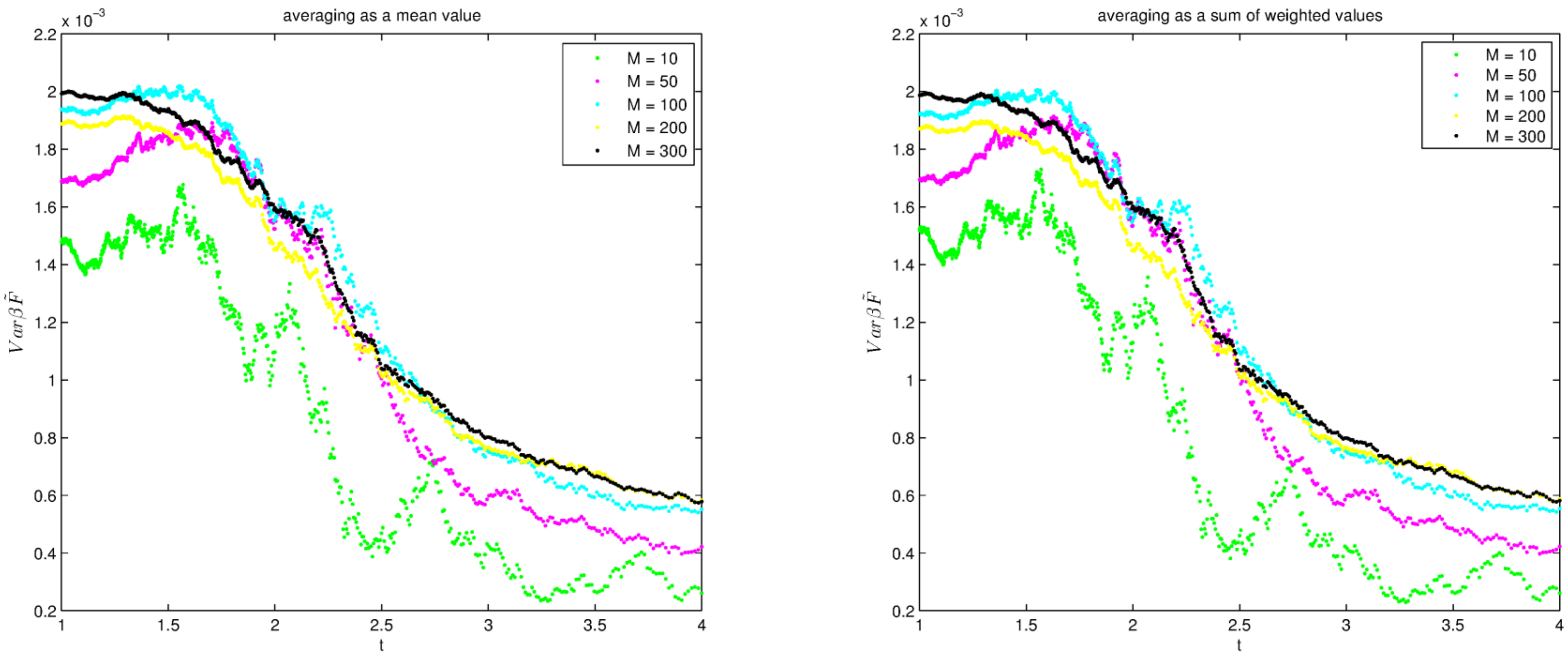
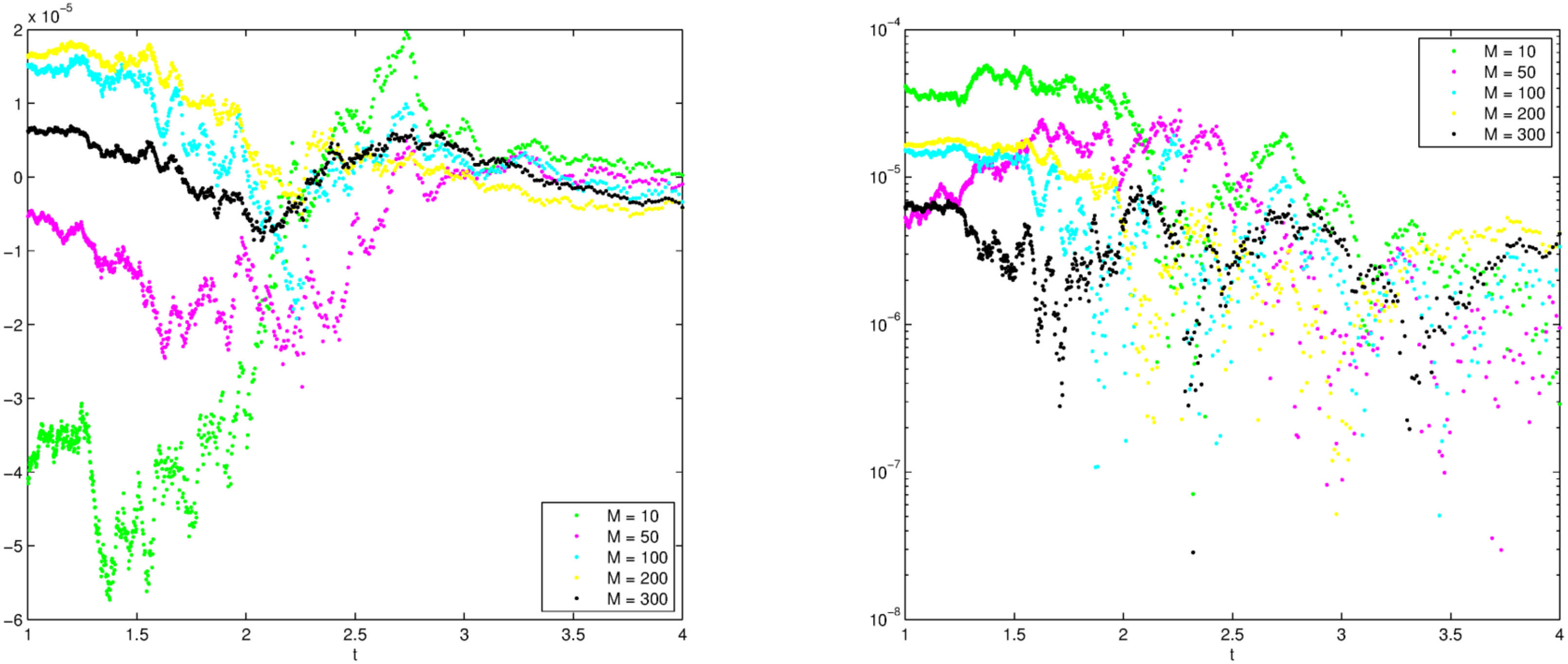


Figure 22a: Heat capacity errors divided by heat capacity as a function of the temperature for a different number of independent runs M.



(a) (b)

Figure 23: Variance of a dimensionless free energy $\beta\tilde{F}$ as a function of temperature for a different number of independent runs M.



(a) difference between values of $\mathrm{Var}\beta\tilde{F}$

(b) absolute difference between values of $\mathrm{Var}\beta\tilde{F}$

Figure 24: Comparison of both cases of calculating the dimensionless free energy variance.

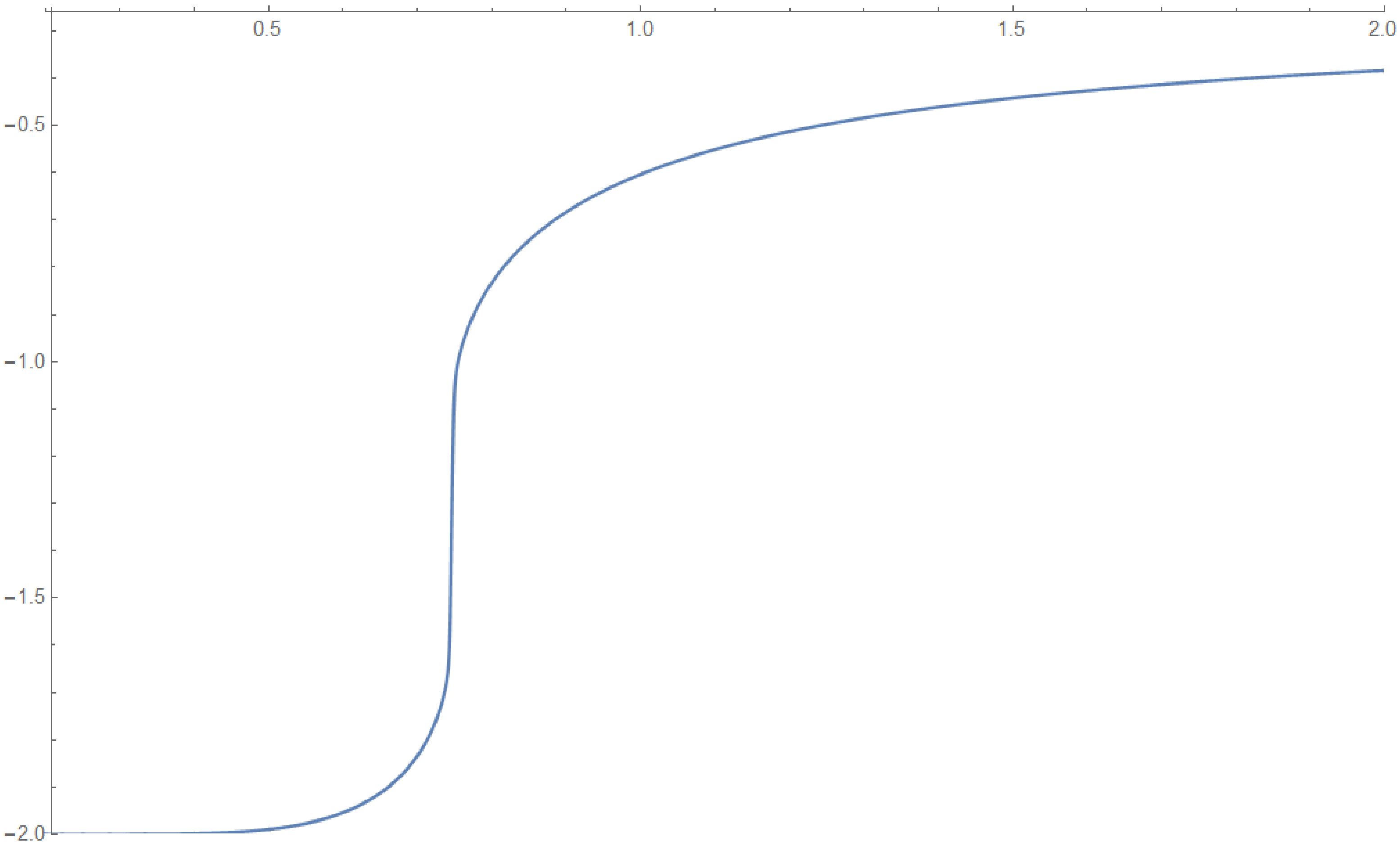


Figure 25: Internal energy as a function of the temperature for 8-state Potts model calculated with Population Annealing for L=32, θ=100, M=200, Δβ=0.001.

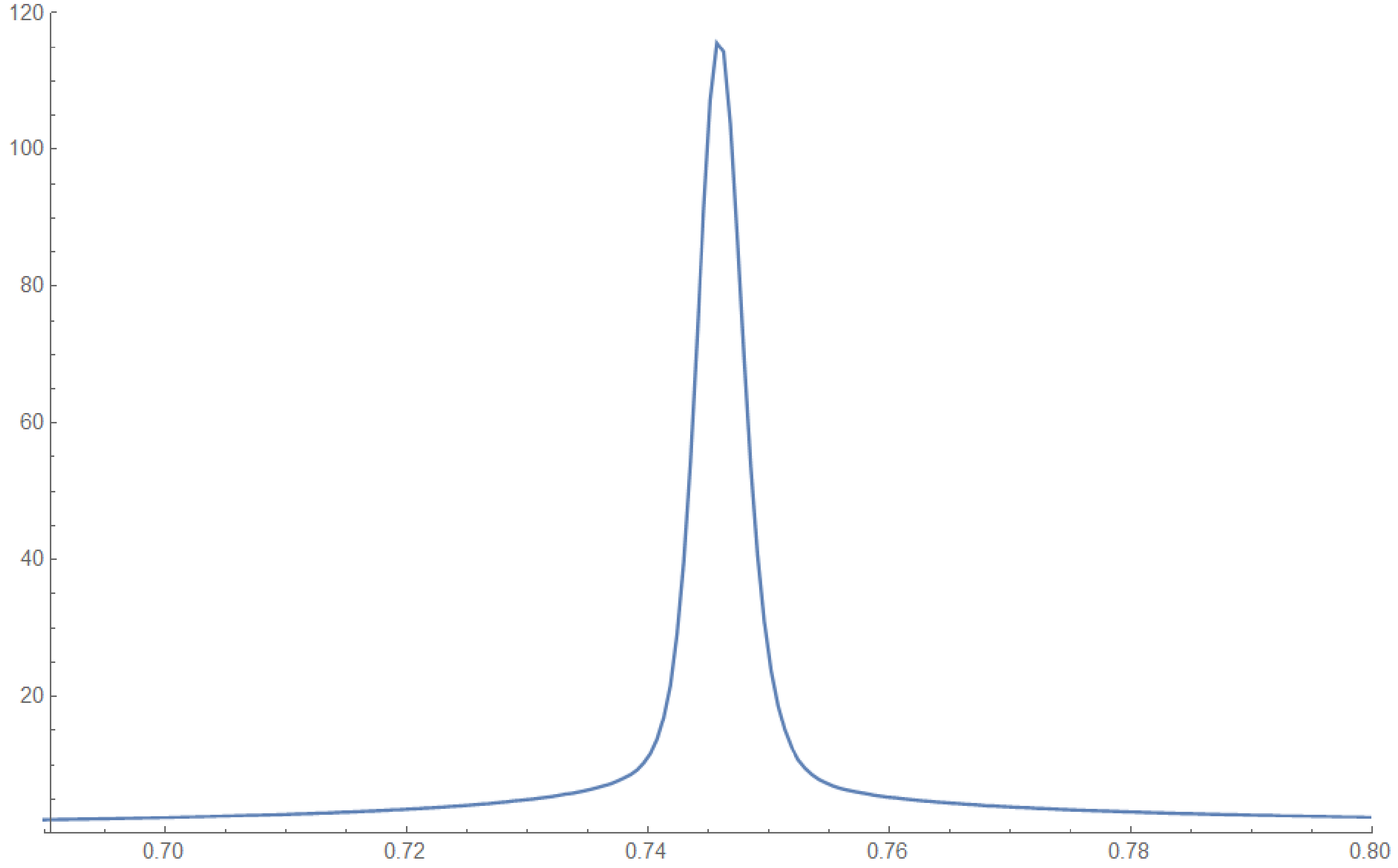


Figure 26: Heat capacity as a function of the temperature for 8-state Potts model calculated with Population Annealing for L=32, θ=100, M=200, Δβ=0.001.