PY421: Assignment #9

Shun Miyamoto
smiyamot@bu.edu

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1 Problem 3

$$
\begin{aligned}
Z &= \sum e^{-\beta E} && (1)\\
< E > &= \frac{\sum E e^{-\beta E}}{\sum e^{-\beta E}} \\
&= -\frac{1}{Z}\frac{\partial Z}{\partial \beta} && (2)\\
&= -\frac{\partial}{\partial \beta}\ln Z && (3)\\
< E^2 > &= \frac{\sum E^2 e^{-\beta E}}{\sum e^{-\beta E}} \\
&= \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} \\
&= \frac{\partial^2}{\partial \beta^2}\ln z + (\frac{\partial}{\partial \beta}\ln Z)^2 && (4)
\end{aligned}
$$

Here, $< E >$ and $< E^2 >$ are for the total number of bonds. Thus, the mean square fluctuation of energy for the total number of bonds is,

$$
\begin{aligned}
C &= < (E- < E >)^2 > \\
&= < E^2 > - < E >^2 \\
&= \frac{\partial^2}{\partial \beta^2}\ln Z \\
&= \frac{\partial}{\partial \beta}(\frac{\partial}{\partial \beta}\ln Z) \\
&= \frac{\partial}{\partial \beta}(\frac{1}{Z}\frac{\partial Z}{\partial \beta}) \\
&= -\frac{\partial}{\partial \beta} < E > && (5)
\end{aligned}
$$

Hence, in our context, it is proved that,

$$C = 2N^2(< E^2 > - < E >^2) = -\frac{\partial}{\partial \beta} < E > \quad (6)$$

2 Problem 4

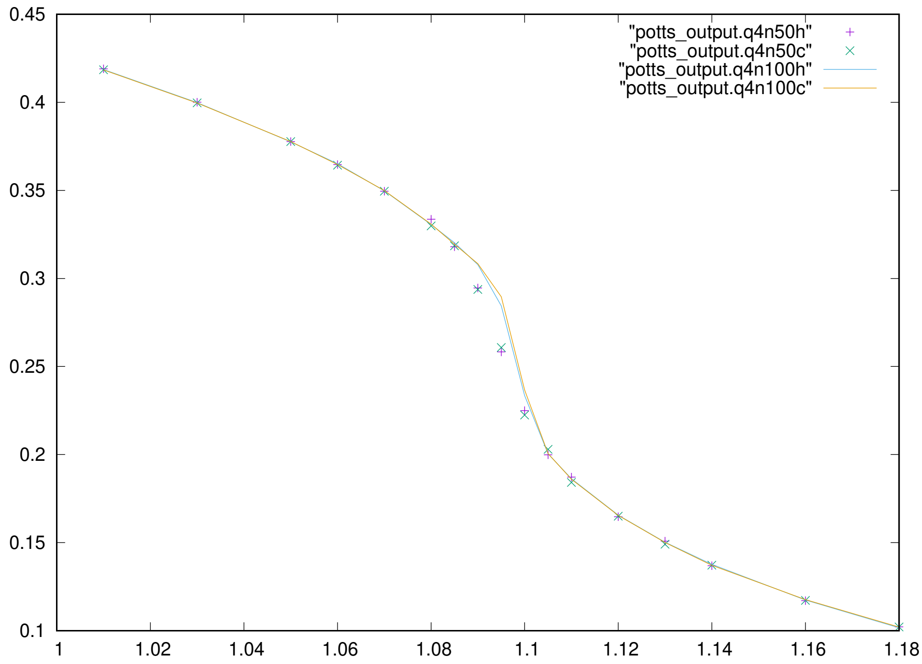

Figure 1: $< E >$ versus β for 4 simulations

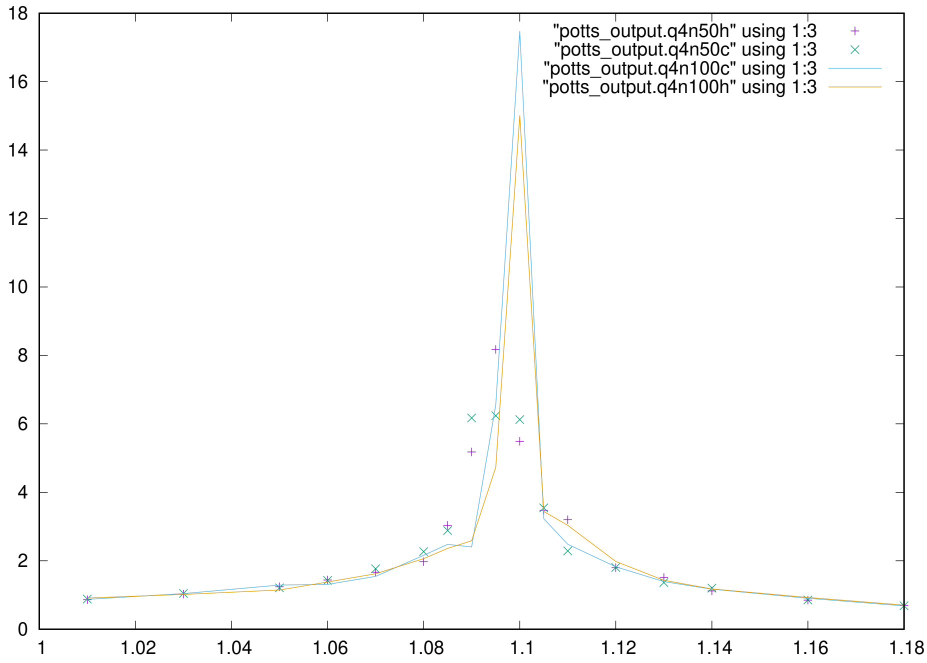

Figure 2: Fluctuation versus β for 4 simulations

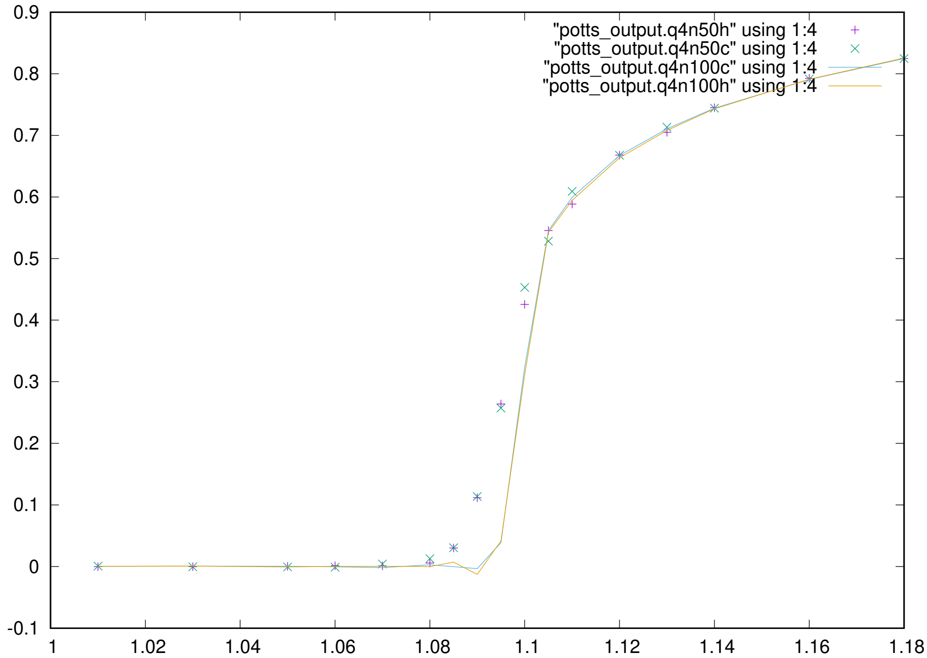

Figure 3: Correlation $< m >$ versus β for 4 simulations

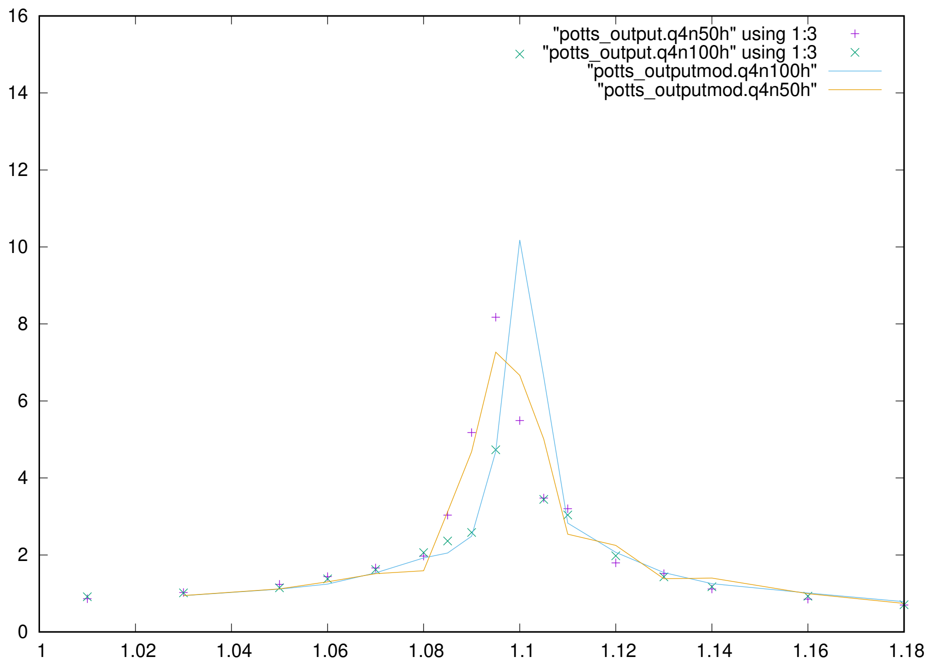

Figure 4: Comparison of values of fluctuation, ones are from simulations, and the others are from approx-iamtion