Computer simulation of physical systems I

Task Vb: Blocking analysis

In this exercise you will learn how to perform blocking analysis. You need to generate a sequence of exponentially correlated Gaussian distributed numbers and then evaluate the statistical error of finite time averages through the blocking method. Executables and sample input files can be found in the archive `taskVb.zip`. Please download the .zip file and unpacked it. The detailed instructions are as follows.

1. Run the python script `stochastic.py` to generate N samples, $\{A_i\}$, with correlation time $\tilde{\tau}$. This script uses the algorithm described in Sec. 5 in `documentation.pdf`. The code also prints out $\langle A \rangle$ and σ_A^2 in the end. Verify $\{A_i\}$ are Gaussian deviates, i.e., $\langle A \rangle = 0$ and $\sigma_A^2 = 1.0$. One can specify N and the correlation time $\tilde{\tau}$ using the variables `nstep` and `tau` in the code, respectively. The generated sequence of exponentially correlated Gaussian distributed numbers is stored in file `DATA.dat`.

2. Calculate $c_{AA}(k)$ by issuing the python script `correlation.py` which reads `DATA.dat` and outputs $c_{AA}(k)$ in file `CORRELATION.dat`. Fit the data with $e^{-|k|/\tau}$ and verify that $\tau = \tilde{\tau}$. `correlation.py` also prints out the integrated $c_{AA}(k)$ using Eq.(13). Verify that the obtained correlation time is equal to $\tilde{\tau}$.

3. Evaluate the statistical error σ_I using Eq. (18).

4. The blocking analysis is done by the python script `blocking.py`. This script reads `DATA.dat` and outputs results in the file `BLOCKING.dat`. The total number of transformation step is controlled by the variable `ntrans`. Use the blocking method and plot $\sigma_I(M)$ as a function of the block transformation step. Evaluate the statistical error at its plateau, $\sigma_I^{plateau}$. Eventually, calculate the ratio $\sigma_I^{plateau}/\sigma_I(0)$ and verify this is equal to $\sqrt{2\tau}$.

5. Use the blocking method, plot $\tau(M)$ and evaluate the correlation time at its plateau $\tau^{plateau}$.

6. At fixed τ, generate different data sequences increasing the number of samples, N. Determine the minimum number of samples that you need for an accurate evaluation of the correlation time and the statistical error. What is the behavior of the statistical error as a function of N ?

7. Calculate σ_I with the blocking analysis for many data set with different correlation time (be sure that $\tau \ll 2^{M_{max}}$ with $M_{max} = log_2 N$). Plot $\sigma_I(\tau)$ as a function of the correlation time and show that $\sigma_I(\tau) = s\sqrt{\frac{2\tau}{N}}$ and $s = \sigma_A$.