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Homework Assignment #1 - Due January 31

Note: When using the "Berkeley Computational Nanoscience Tool Kit" tool and running the "Average" simulation, all of the simulations you execute will remain in memory for a given tool session. Therefore, we recommend launching the tool once for the first data set, and then closing and restarting for the second data set, and so forth.

ERROR BARS

Files [d1.dat](#), [d2.dat](#) and [d3.dat](#) contain the results of the first M estimates of arbitrary physical quantities, referred to as \mathbf{A} , obtained in three different computer simulations. The purpose of this exercise is to use the simulation data to obtain a reliable estimate of the average value of the quantity of interest and of its statistical uncertainty (one standard deviation).

In order to do this, we will use the simple FORTRAN code ingeniously called average (which can be found in the class [nanoHUB](#) toolkit).

These are plots referring to the three different data files; they show features which occur in almost all simulations, namely :

- i) the first few data points are contaminated by the initial conditions of the simulation.
- ii) there is autocorrelation between nearby data points even when the system has settled down.

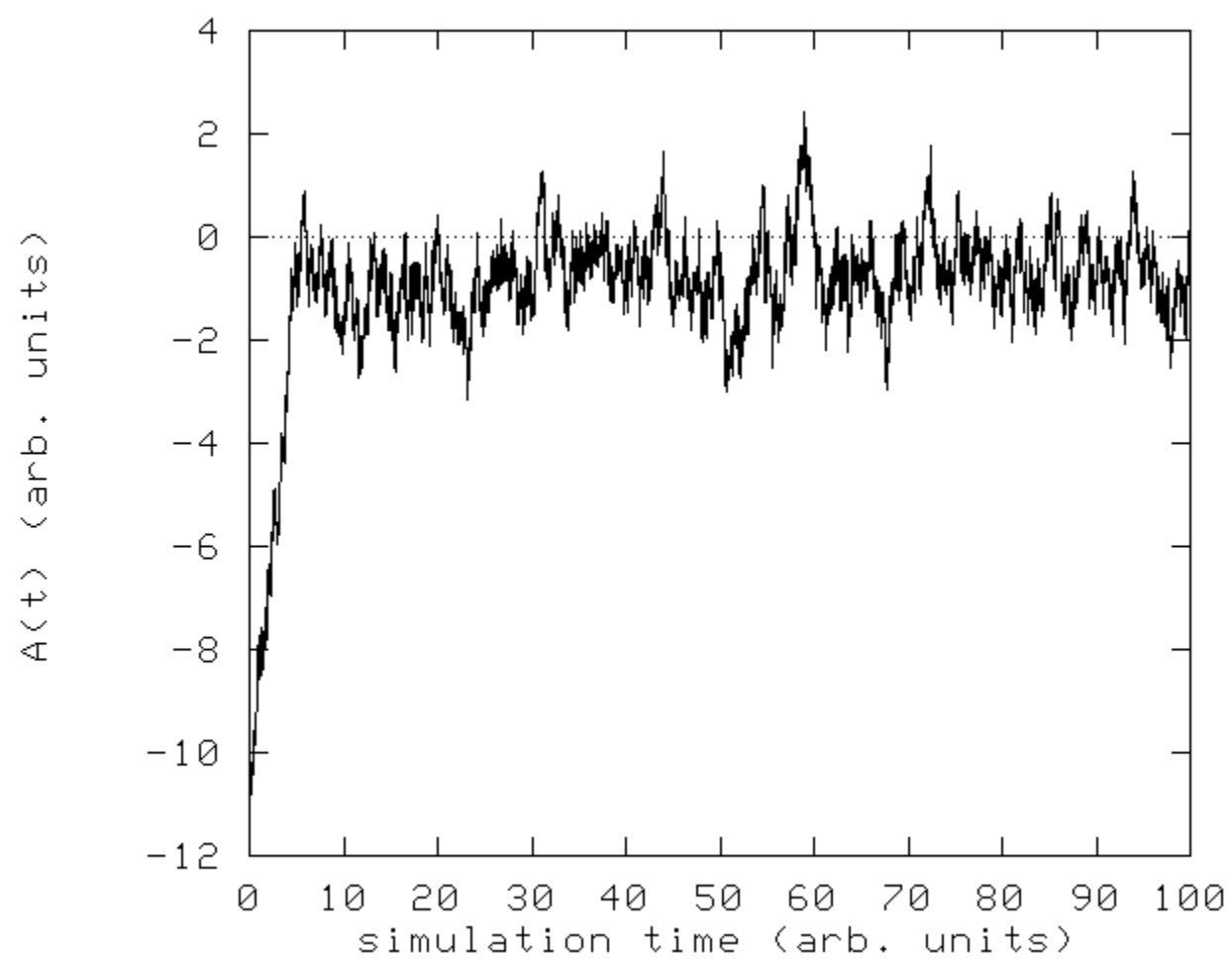


Fig.1 File d1.dat

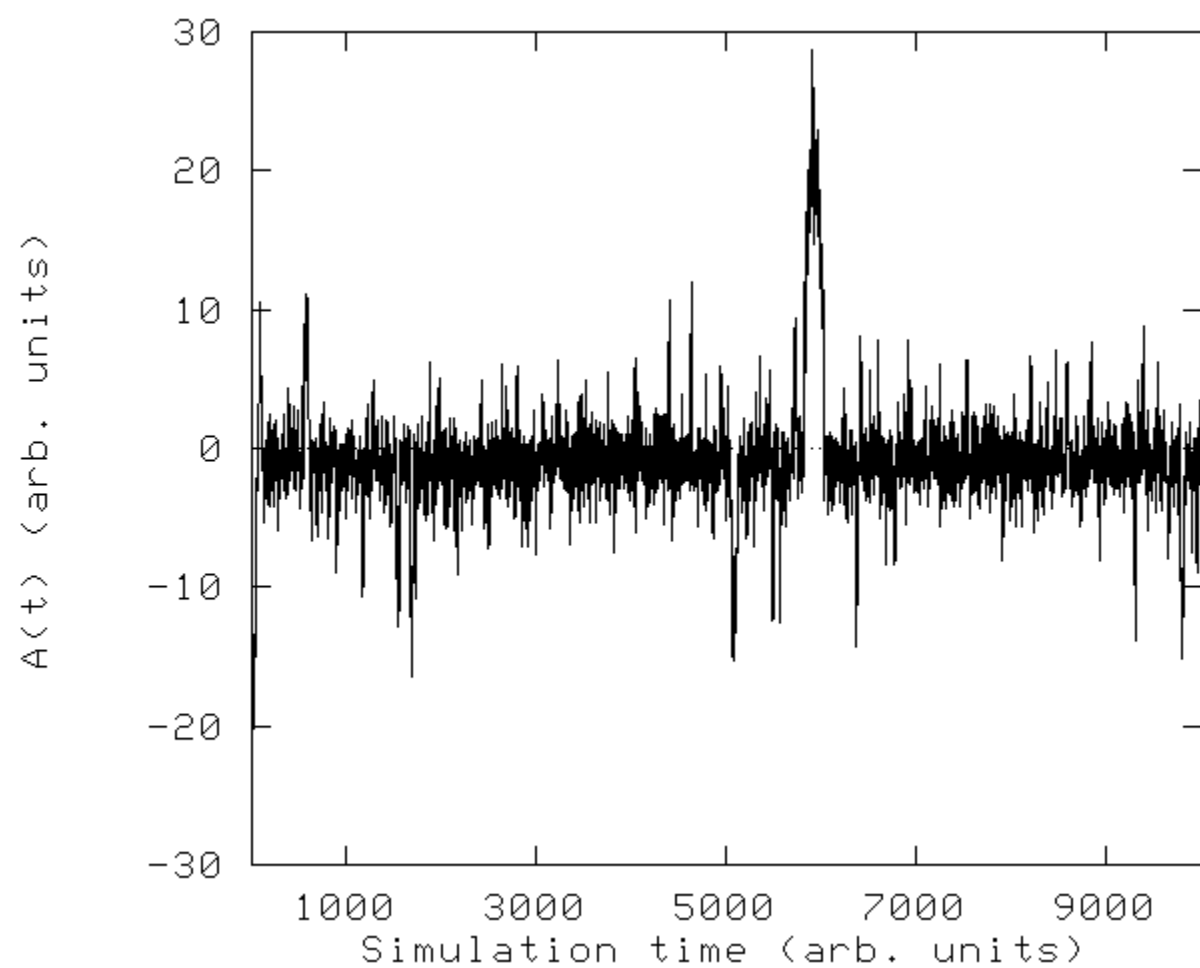


Fig.2 File d2.dat

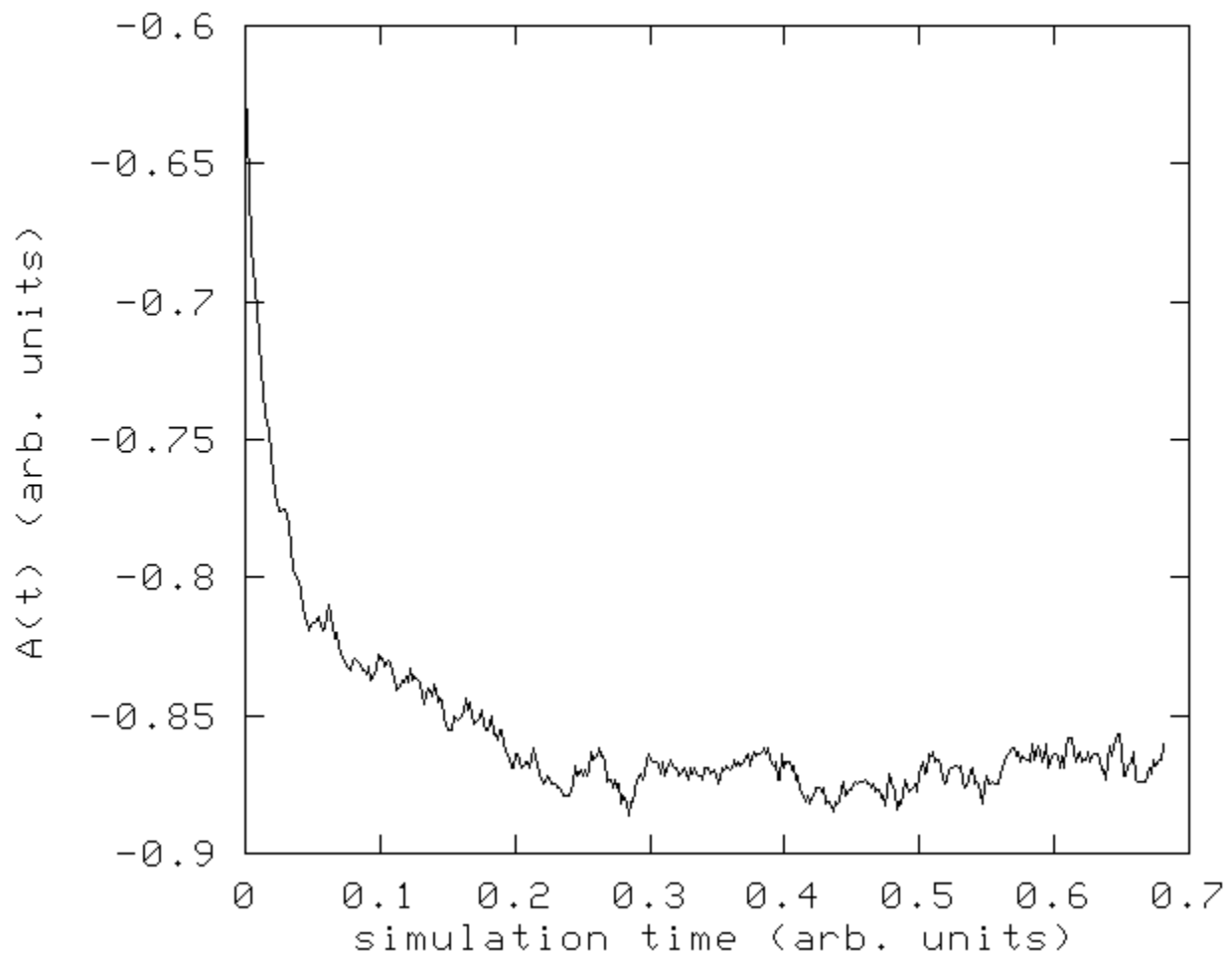


Fig.3 File d3.dat

Using the average program, estimate for the three above cases

- The average value of the plotted quantity: How many initial data points must be discarded ?
 - The statistical error of : is the **fixed point** of the blocking transformation reached? If so, at which bin length?
 - Which simulation, according to you, needs to be run for a longer time?
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