Worksheet 4: Error Analysis and Langevin Thermostat

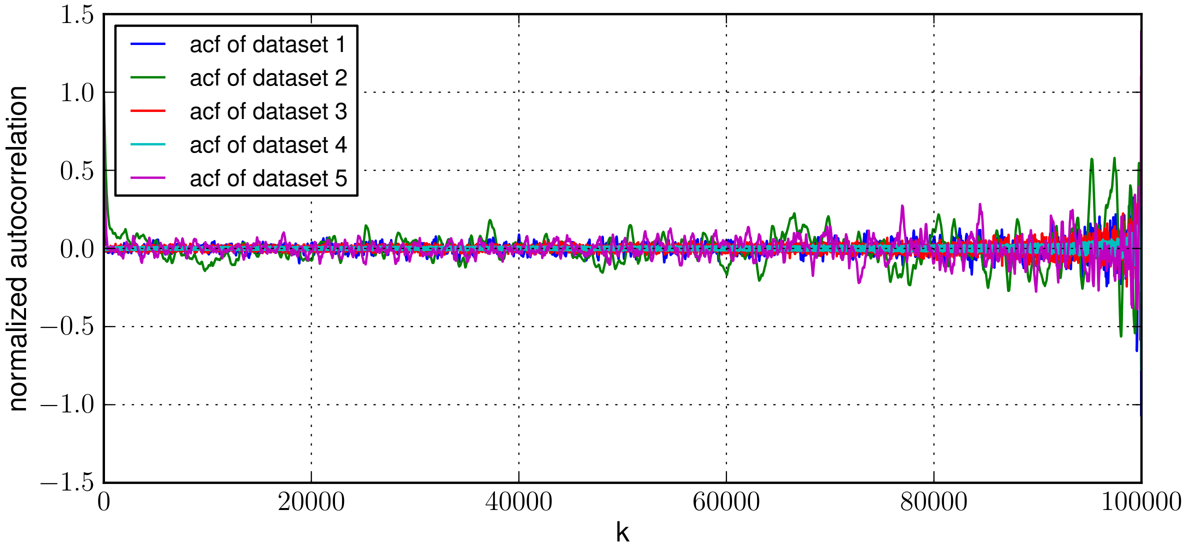
April Cooper, Patrick Kreissl und Sebastian Weber

January 10, 2013
University of Stuttgart

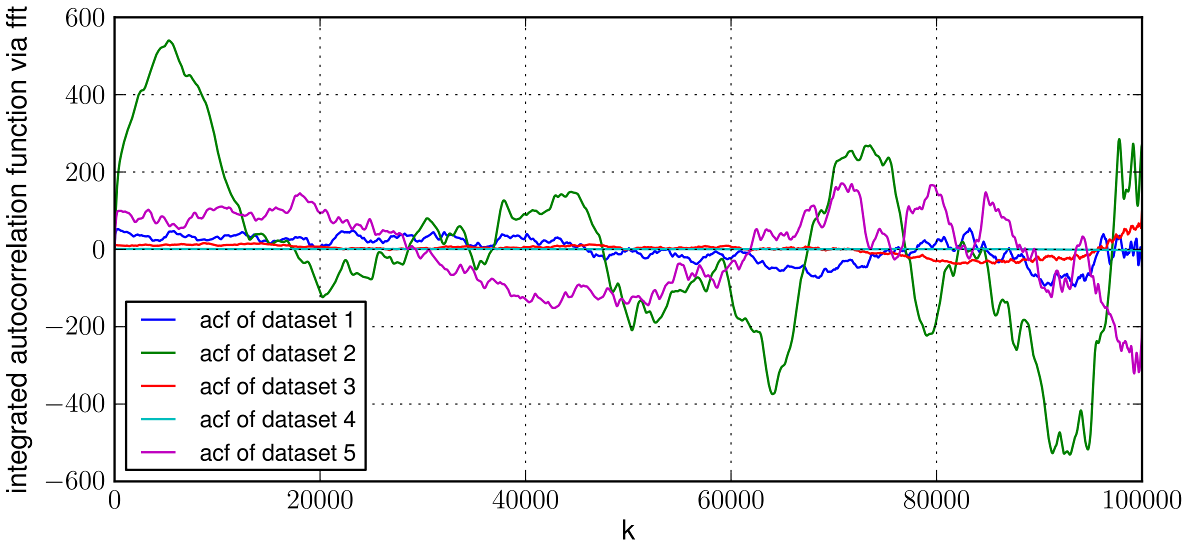
1 Error Analysis

1.1 Autocorrelation Analysis

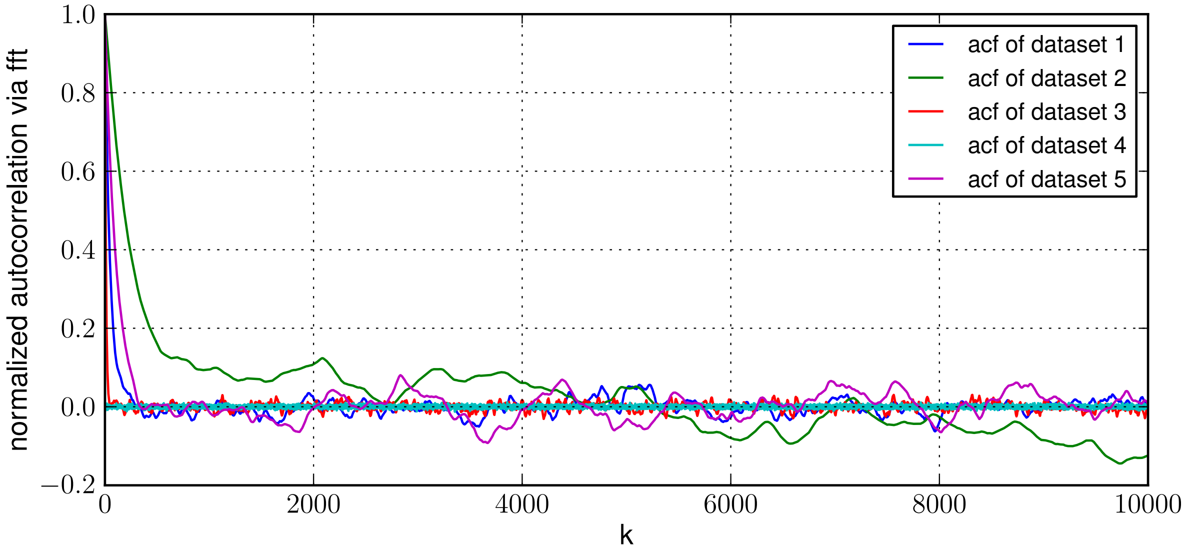
In this section we had to implement a Python function that computes the autocorrelaton function of a given time series and use this function on the given datasets. The resulting plot can be seen below:

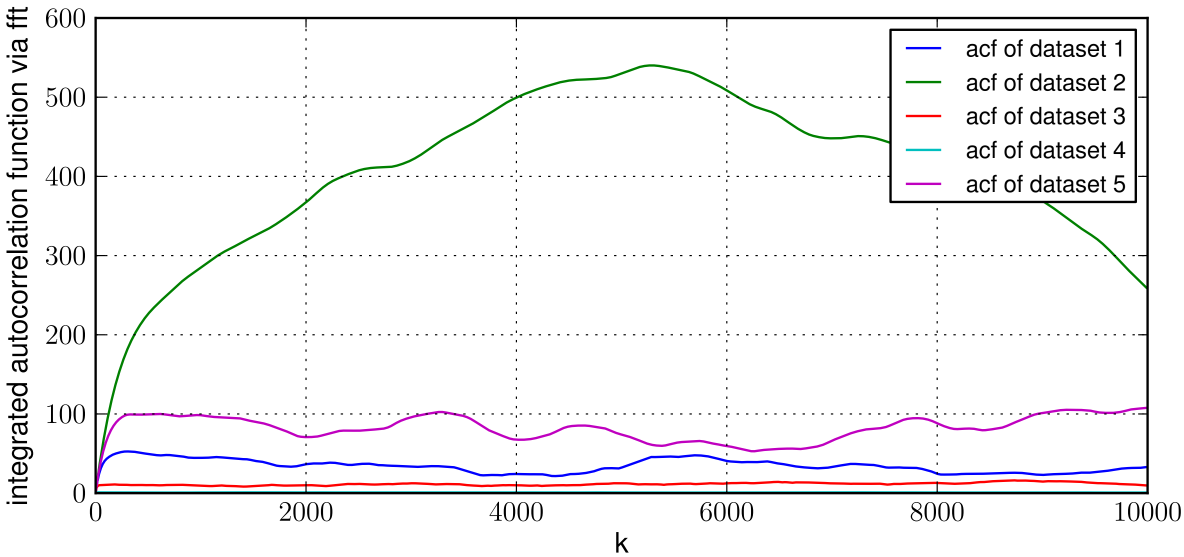


Furthermore we were supposed to plot the integrated autocorrelation function which can be seen below:



As you can see in the plots, it is not useful to integrate the function over the whole interval because the lager the autocorellations shift parameter k becomes the lareger the fluctuation of the autocorrelation function becomes. This is because for larger ks due to the autocorrelations definition less data is used to compute the function. Therefore the statistical fluctuation of a single datapoint has more influence on the computed autocorrelation function. This larger fluctuation influences also manifest in the integrated autocorrelation function. The integrated function should converge against the autocorrelation time. So for a visual estimate of the autocorrelation time the only relevant part of the interval is the one in which the autocorrelation funcion approximately acts like an exponetial function and where the influence of the intrisic error of the function due to the increased influence of statistical fluctuations is still relatively small. In the following plots we zoomed in to the relevant interval:





The autocorrelation times of the datasets can be visually guessed as follows:

dataset	guessed autocorrelation time
1	50
2	450
3	10
4	1
5	90

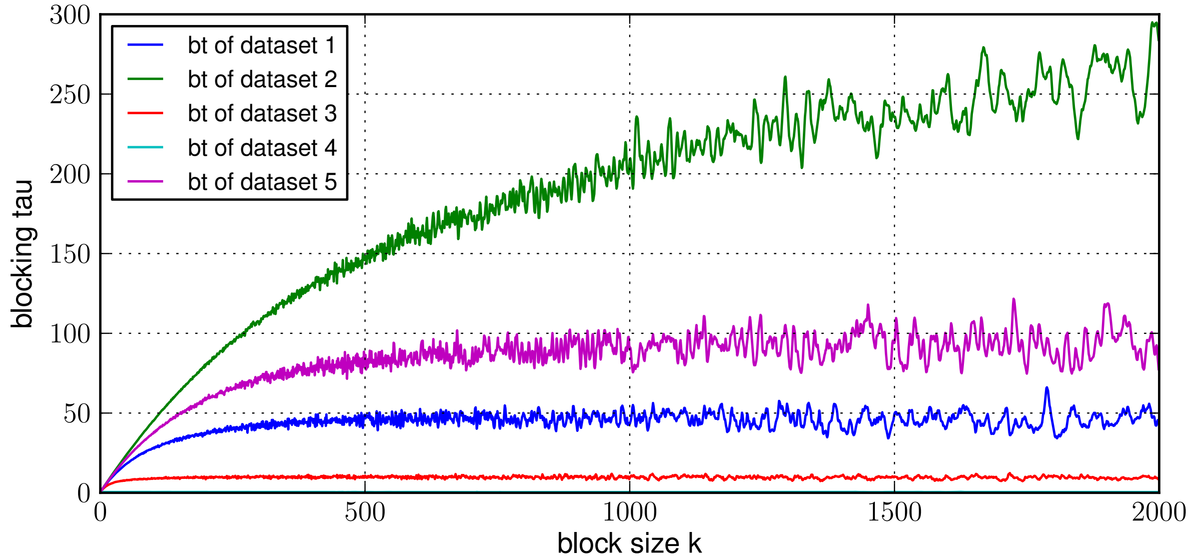
The next task was to implement a Python function that performs automatic error analysis via autocorrelation analysis of a given time series of an observable. This function should compute an estimate of the outocorrelation time via the running autocorrelation time estimator, where the integration is cut of when $k_{\max} \geq 6\hat{\tau}_{\mathcal{O},\text{int}}(k_{\max})$. The function was supposed to return the mean value of the observable $\bar{\mathcal{O}}$, the error of the mean value $\epsilon_{\bar{\mathcal{O}}}$, the estimated autocorrelation time $\hat{\tau}_{\mathcal{O},\text{int}}$, its error $\epsilon_{\hat{\tau}_{\mathcal{O},\text{int}}}$ and the effective statistics N_{eff}. The results shown in the folowing table:

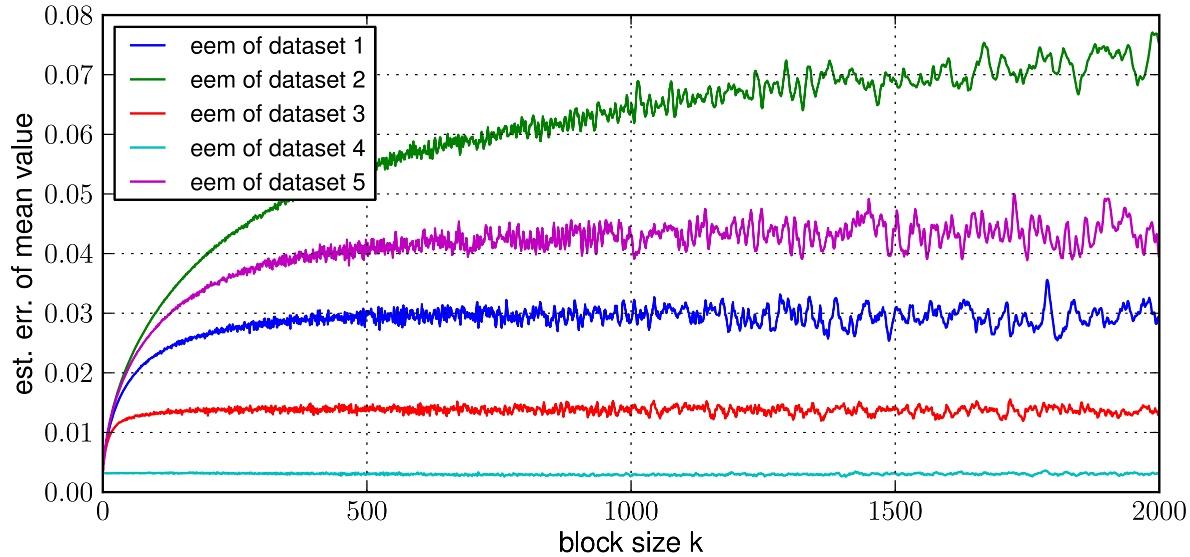
dataset	$\bar{\mathcal{O}}$	$\epsilon_{\bar{\mathcal{O}}}$	$\hat{\tau}_{\mathcal{O},\text{int}}$	$\epsilon_{\hat{\tau}_{\mathcal{O},\text{int}}}$	N_{eff}
1	$8.2468 \cdot 10^{-15}$	0.0031	52.134	5.8381	956
2	$3.9756 \cdot 10^{-14}$	0.0032	403.139	125.4145	123
3	$4.0010 \cdot 10^{-15}$	0.0031	9.707	0.4736	5042
4	$-1.4214 \cdot 10^{-13}$	0.0032	0.5039	0.0068	66666
5	$-3.1724 \cdot 10^{-14}$	0.0032	99.4101	15.3684	502

As you can see the visually estimated autocorrelation times are very similar to the computed ones. The dataset for witch it was most difficult to guess the autocorrelation time was dataset 2. This manifests in the computed error of the autocorrelation time of that dataset, too. It is nearly by factor 10 larger than the error of dataset 5, and even by factor 100 for the datasets 3 and 4.

1.2 Binning Analysis

We were supposed to implement a Python function that computes the block variance σ_B^2 for a given block size k. From that block variance the estimated autocorrelation time $\tau_{\mathcal{O},\text{int}}$ and error of the mean value $\epsilon_{\bar{\mathcal{O}}}$ can be computed. Our task was to plot theese for $1 < k < 2000$. The resulting plots are shown below:





From the plots the autocorrelation time and the error of the mean value can be guessed as follows:

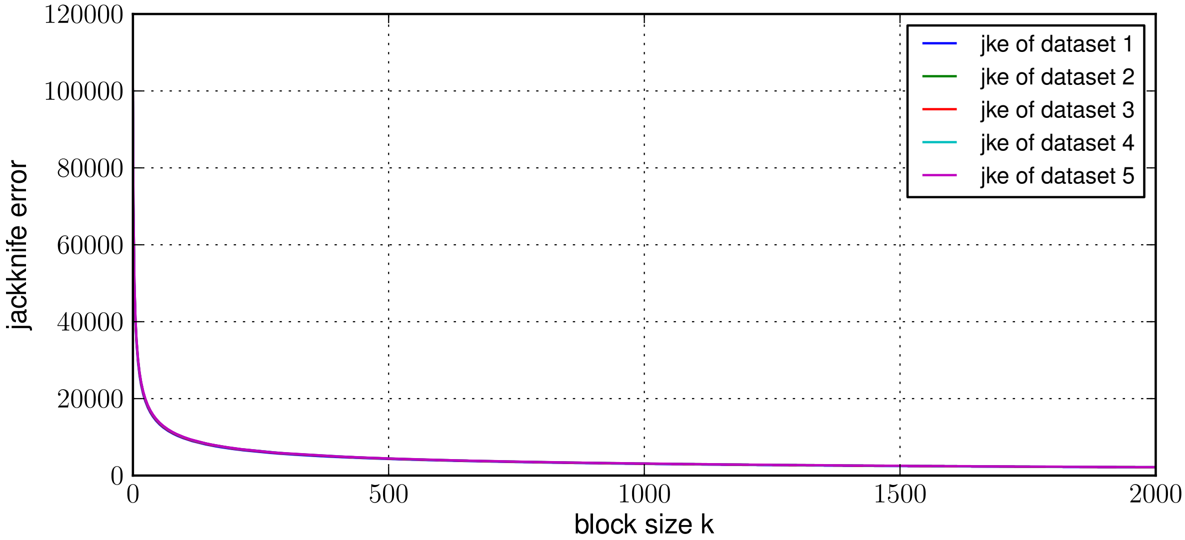
dataset	$\tau_{\mathcal{O},\text{int}}$	$\epsilon_{\bar{\mathcal{O}}}$
1	49	0,030
2	-	-
3	10	0,014
4	1	0,004
5	90	0.042

For both, autocorrelation time and the error of the mean value, for dataset 2 at the end of the interval ($k = 2000$) the functions do still not converge, while the fluctuation of the data becomes already relatively large. Therefore for dataset 2 no values could be estimated.
For the others the autocorrelation time matches the values obtained in the previous tasks.

For the error of the mean value only the error of dataset 1 matches the previous estimated value. The error of the other is smaller than previously obtained.

1.3 Jackknife Analysis

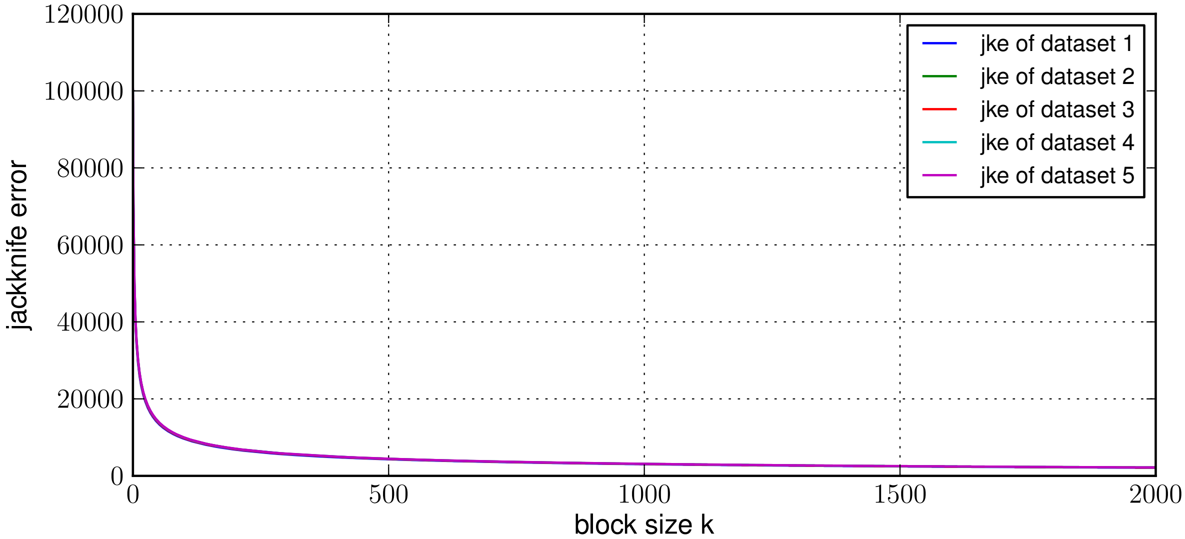
In this section we had to implement a Python funcion that computes the Jackknife error $\epsilon_{\bar{O}}$ for a given time series and block size k. The resulting plot is shown below:



The computed errors would range from 2126 to 2203 at $k = 2000$. That seems hardly plausible and does not match the values obtained in the other tasks at all.

1.4 Jackknife Analysis

In this section we had to implement a Python funcion that computes the Jackknife error $\epsilon_{\bar{O}}$ for a given time series and block size k. The resulting plot is shown below:



The computed errors would range from 2126 to 2203 at $k = 2000$. That seems hardly plausible and does not match the values obtained in the other tasks at all.

2 Error Analysis of Real Simulation Data

2.1 Langevin Thermostat

The Langevin Thermostat was implemented according to the following formula [1] (in reduced units):

$$F = -\nabla U(x) - \gamma v + \sqrt{2\gamma \cdot T} \cdot R(t) \tag{1}$$

R(t) is a delta-correlated stationary Gaussian process with zero-mean, for example white noise. As an approximation Gaussian noise with mean = 0 and variance = 1 was used. Furthermore it was necessary to multiply the values of the generated noise by ten to get the right temperatures. This points to a possible error.

The function was written in the python part because no loops or other time consuming stuff was needed - except for the noise generation that was done by a fast numpy function.

As a result we got the following equilibrium mean values

The averages were taken from t = 700 to t = 1000.
For T = 0.3 (measurement 0.302)

- pressure $p = -0.0903$, potential energy per particle $E_{pot} = -5.74$

For T = 1.0 (measurement 1.004)

- pressure $p = 0.0624$, potential energy per particle $E_{pot} = -2.48$

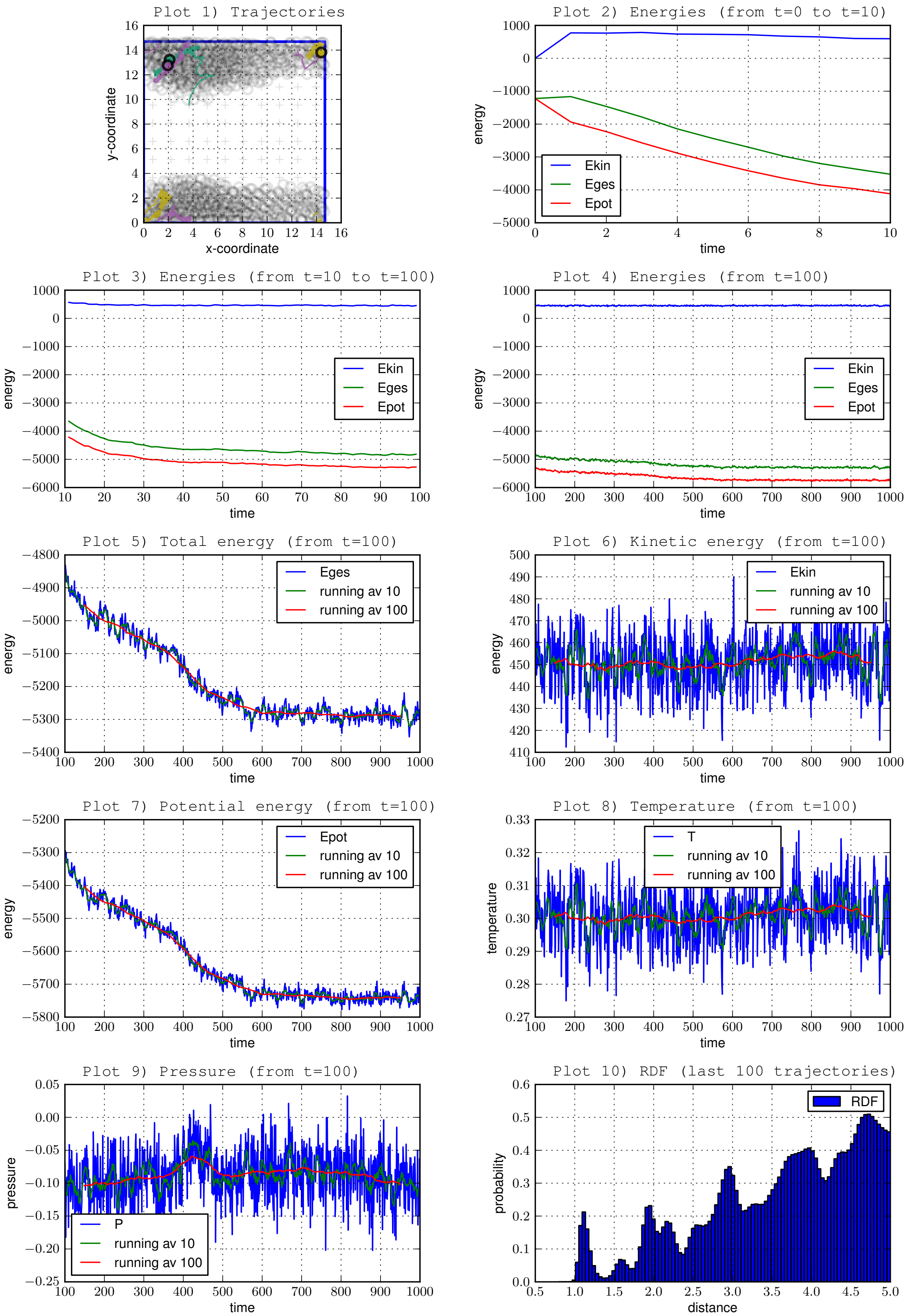
For T = 2.0 (measurement 2.018)

- pressure $p = 0.6319$, potential energy per particle $E_{pot} = -1.69$

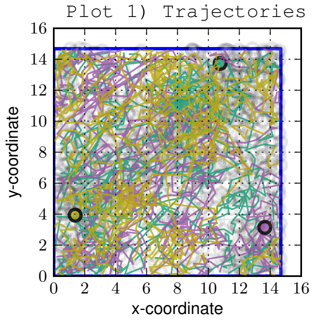
[1] source:http://en.wikipedia.org/wiki/Langevin_dynamics, visited on January 9, 2013

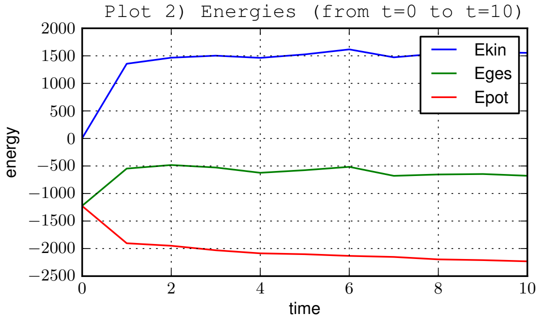
2.2 Plots

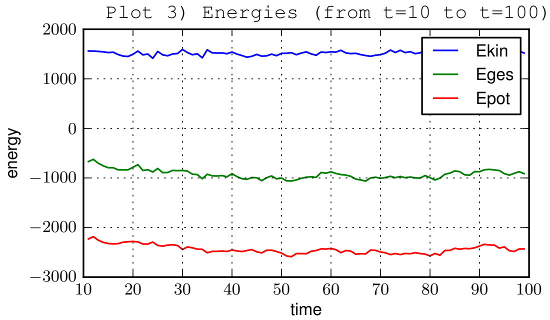
For T=0.3

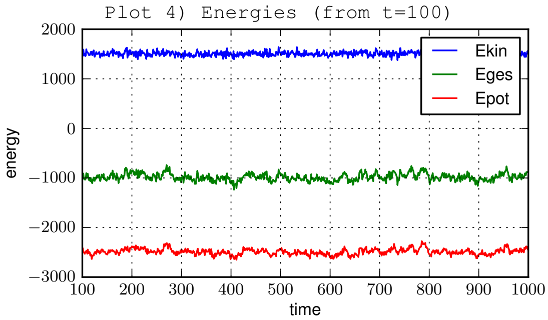


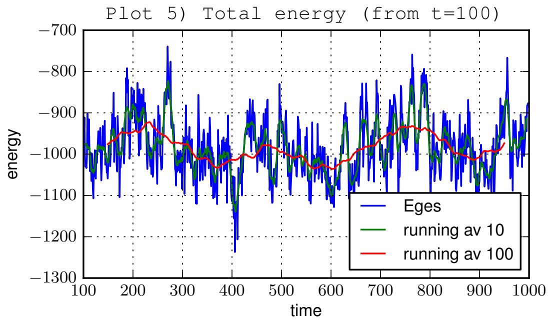
For T=1.0

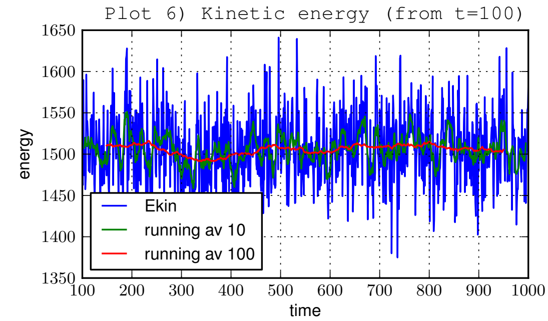

Plot 1) Trajectories
y-coordinate
x-coordinate

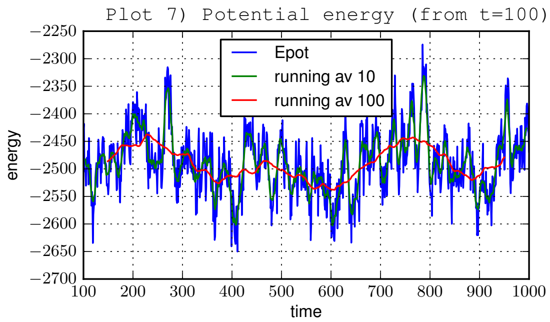

Plot 2) Energies (from t=0 to t=10)
energy
time
Ekin
Eges
Epot

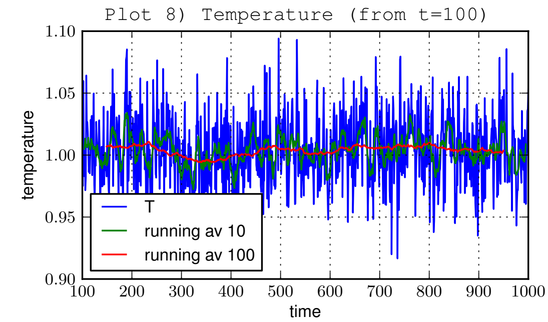

Plot 3) Energies (from t=10 to t=100)
energy
time
Ekin
Eges
Epot

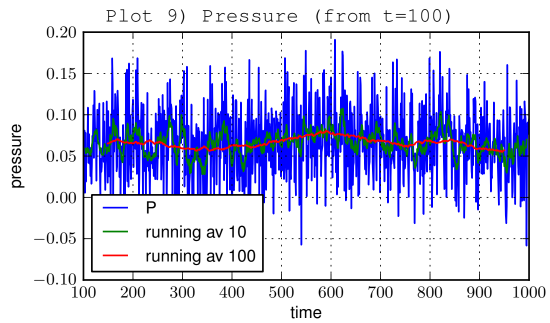

Plot 4) Energies (from t=100)
energy
time
Ekin
Eges
Epot

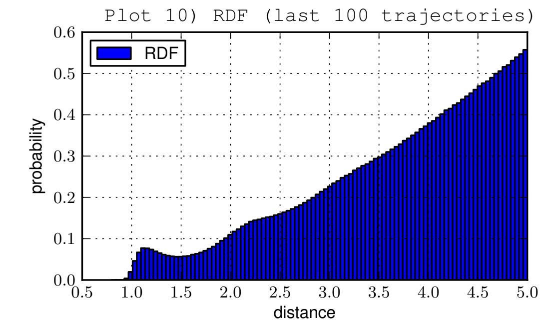

Plot 5) Total energy (from t=100)
energy
time
Eges
running av 10
running av 100


Plot 6) Kinetic energy (from t=100)
energy
time
Ekin
running av 10
running av 100

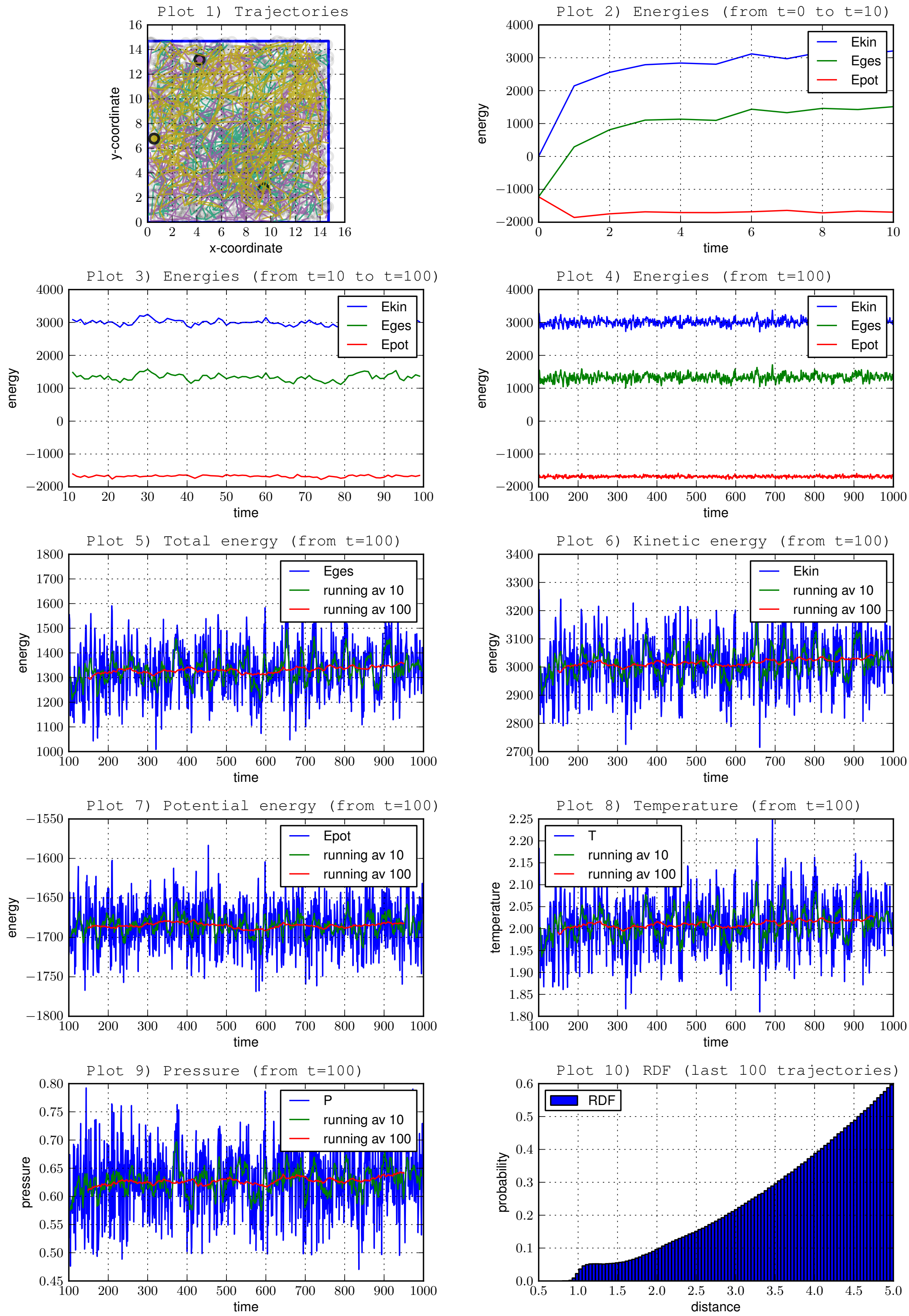

Plot 7) Potential energy (from t=100)
energy
time
Epot
running av 10
running av 100


Plot 8) Temperature (from t=100)
temperature
time
T
running av 10
running av 100


Plot 9) Pressure (from t=100)
pressure
time
P
running av 10
running av 100

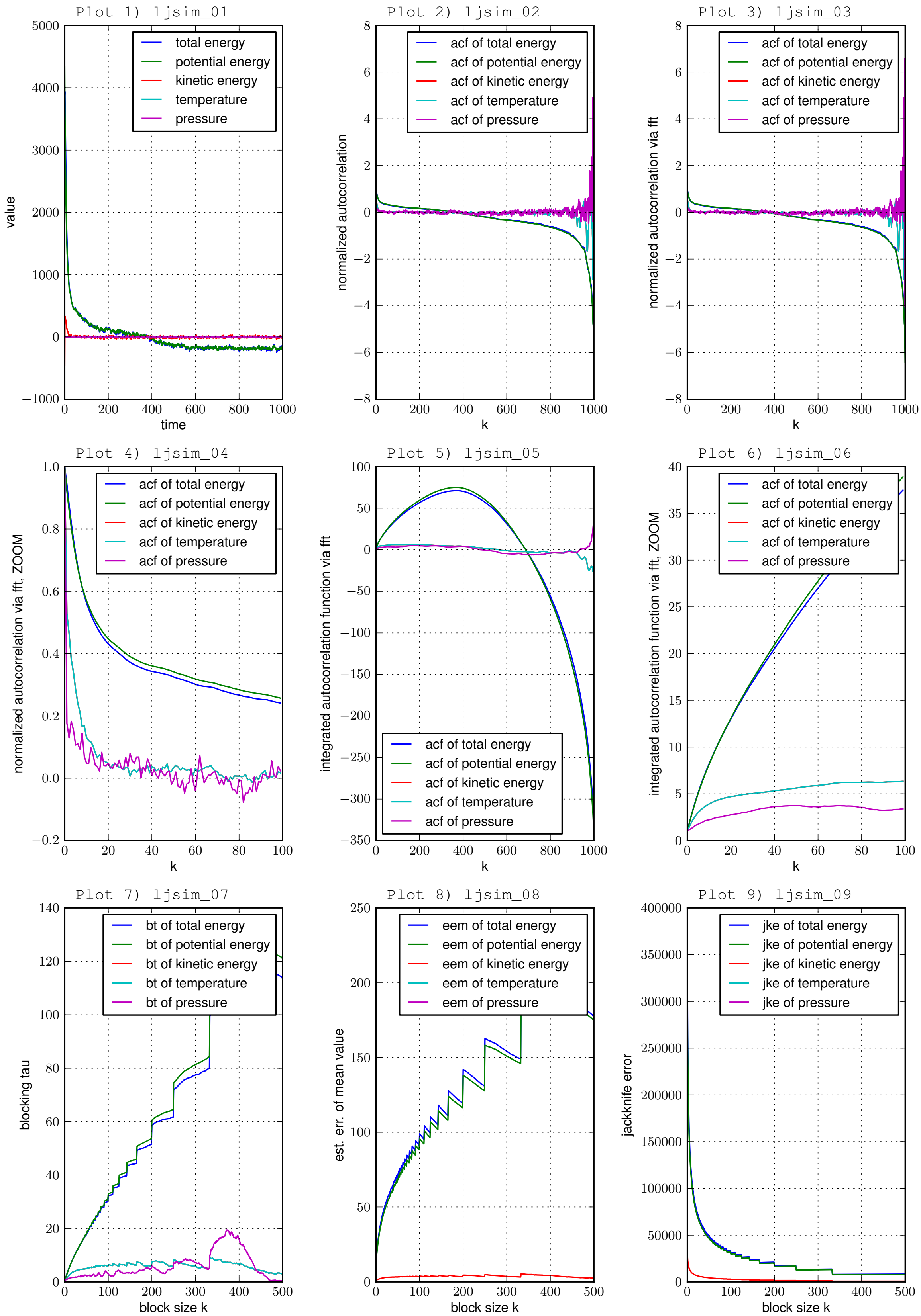

Plot 10) RDF (last 100 trajectories)
probability
distance
RDF

For T=2.0

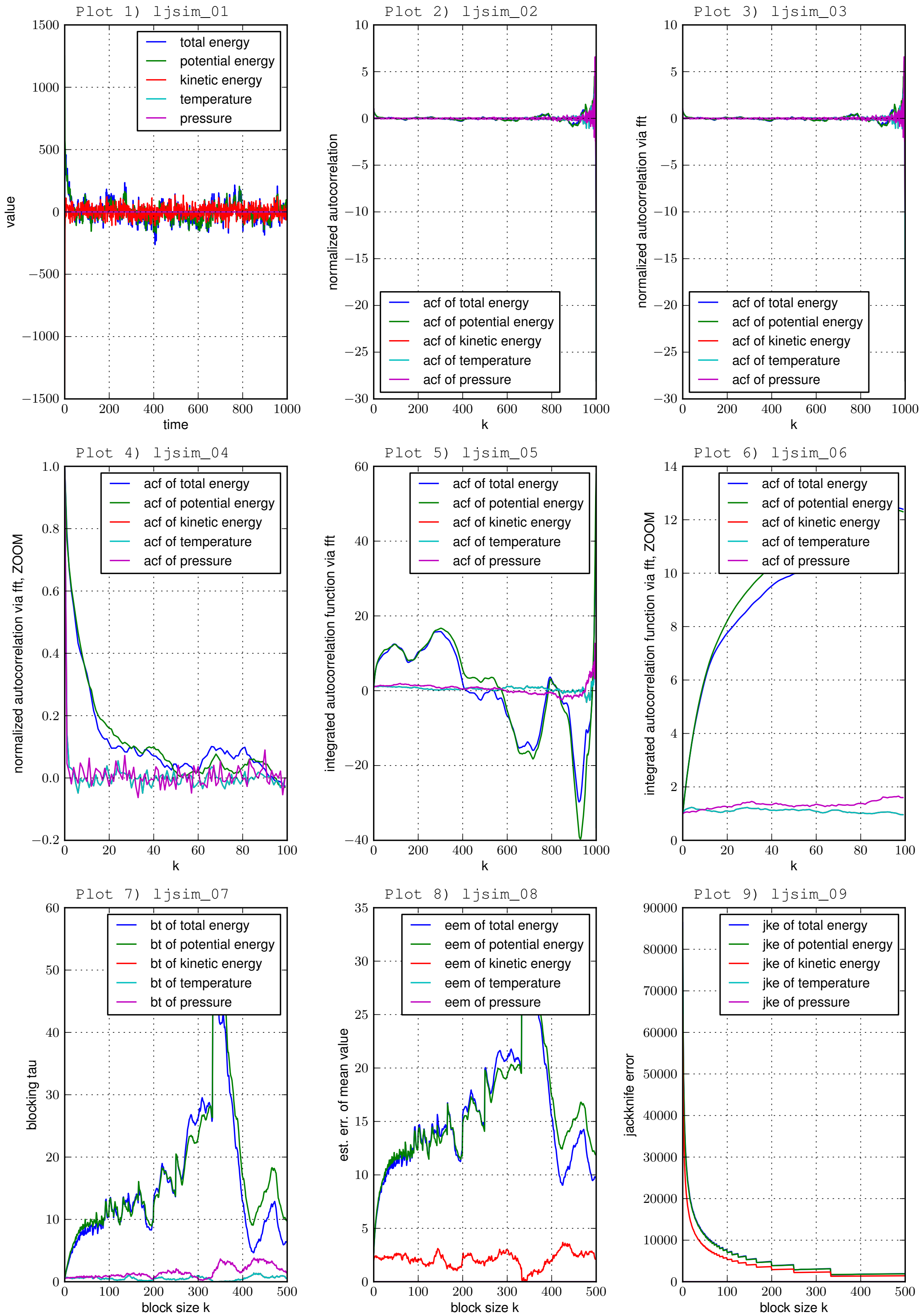

Plot 1) Trajectories
y-coordinate
x-coordinate
Plot 2) Energies (from t=0 to t=10)
energy
time
Ekin
Eges
Epot
Plot 3) Energies (from t=10 to t=100)
energy
time
Ekin
Eges
Epot
Plot 4) Energies (from t=100)
energy
time
Ekin
Eges
Epot
Plot 5) Total energy (from t=100)
energy
time
Eges
running av 10
running av 100
Plot 6) Kinetic energy (from t=100)
energy
time
Ekin
running av 10
running av 100
Plot 7) Potential energy (from t=100)
energy
time
Epot
running av 10
running av 100
Plot 8) Temperature (from t=100)
temperature
time
T
running av 10
running av 100
Plot 9) Pressure (from t=100)
pressure
time
P
running av 10
running av 100
Plot 10) RDF (last 100 trajectories)
probability
distance
RDF

2.3 Error Analysis

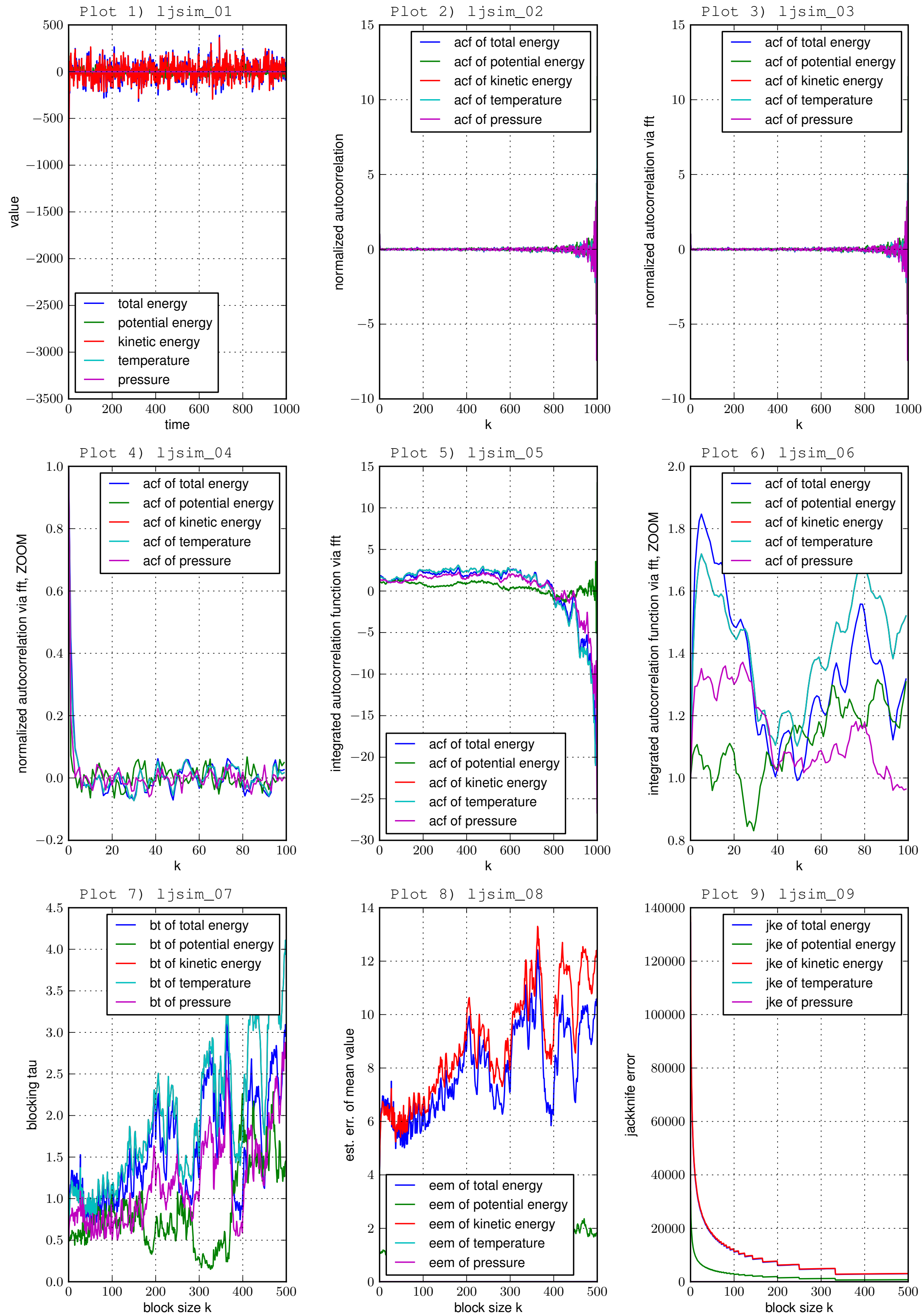
For T=0.3



For T=1.0


Plot 1) ljsim_01
value
time
total energy
potential energy
kinetic energy
temperature
pressure
Plot 2) ljsim_02
normalized autocorrelation
k
acf of total energy
acf of potential energy
acf of kinetic energy
acf of temperature
acf of pressure
Plot 3) ljsim_03
normalized autocorrelation via fft
k
acf of total energy
acf of potential energy
acf of kinetic energy
acf of temperature
acf of pressure
Plot 4) ljsim_04
normalized autocorrelation via fft, ZOOM
k
acf of total energy
acf of potential energy
acf of kinetic energy
acf of temperature
acf of pressure
Plot 5) ljsim_05
integrated autocorrelation function via fft
k
acf of total energy
acf of potential energy
acf of kinetic energy
acf of temperature
acf of pressure
Plot 6) ljsim_06
integrated autocorrelation function via fft, ZOOM
k
acf of total energy
acf of potential energy
acf of kinetic energy
acf of temperature
acf of pressure
Plot 7) ljsim_07
blocking tau
block size k
bt of total energy
bt of potential energy
bt of kinetic energy
bt of temperature
bt of pressure
Plot 8) ljsim_08
est. err. of mean value
block size k
eem of total energy
eem of potential energy
eem of kinetic energy
eem of temperature
eem of pressure
Plot 9) ljsim_09
jackknife error
block size k
jke of total energy
jke of potential energy
jke of kinetic energy
jke of temperature
jke of pressure

For T=2.0


Plot 1) ljsim_01
value
time
total energy
potential energy
kinetic energy
temperature
pressure
Plot 2) ljsim_02
normalized autocorrelation
k
acf of total energy
acf of potential energy
acf of kinetic energy
acf of temperature
acf of pressure
Plot 3) ljsim_03
normalized autocorrelation via fft
k
acf of total energy
acf of potential energy
acf of kinetic energy
acf of temperature
acf of pressure
Plot 4) ljsim_04
normalized autocorrelation via fft, ZOOM
k
acf of total energy
acf of potential energy
acf of kinetic energy
acf of temperature
acf of pressure
Plot 5) ljsim_05
integrated autocorrelation function via fft
k
acf of total energy
acf of potential energy
acf of kinetic energy
acf of temperature
acf of pressure
Plot 6) ljsim_06
integrated autocorrelation function via fft, ZOOM
k
acf of total energy
acf of potential energy
acf of kinetic energy
acf of temperature
acf of pressure
Plot 7) ljsim_07
blocking tau
block size k
bt of total energy
bt of potential energy
bt of kinetic energy
bt of temperature
bt of pressure
Plot 8) ljsim_08
est. err. of mean value
block size k
eem of total energy
eem of potential energy
eem of kinetic energy
eem of temperature
eem of pressure
Plot 9) ljsim_09
jackknife error
block size k
jke of total energy
jke of potential energy
jke of kinetic energy
jke of temperature
jke of pressure