Worksheet 4: Error Analysis and Langevin Thermostat

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Contents

1 Error Analysis

1.1 Langevin Thermostat

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

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

R(t) should be 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 $E_{pot} = -2.48$

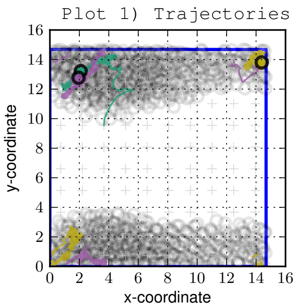
For T = 2.0 (measurement 2.018)

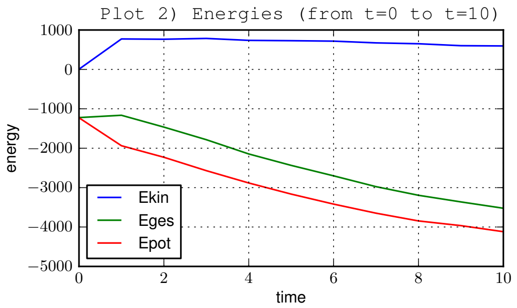
- pressure $p = 0.6319$, potential energy per particle $E_{pot} = -1.69$

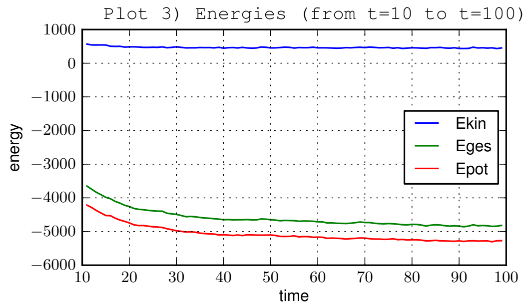
[1] source:`http://en.wikipedia.org/wiki/Langevin_dynamics`, visited on January 9, 2013

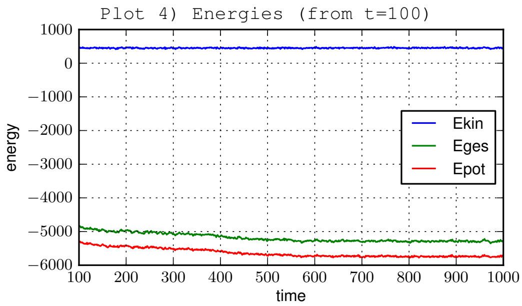
Plots

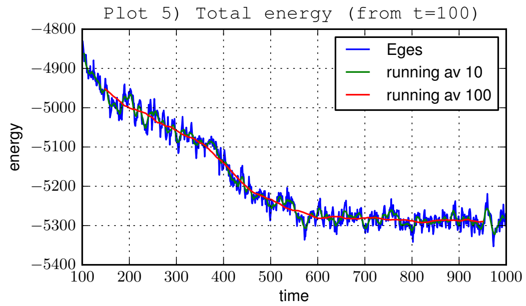
For T=0.3

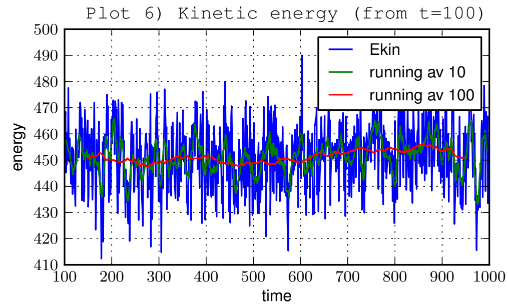


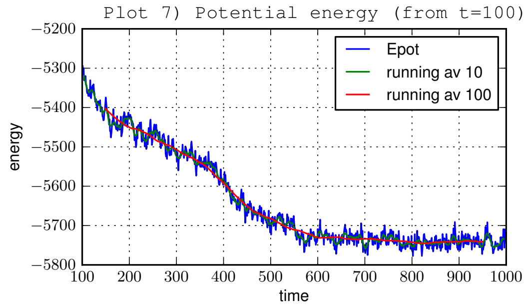


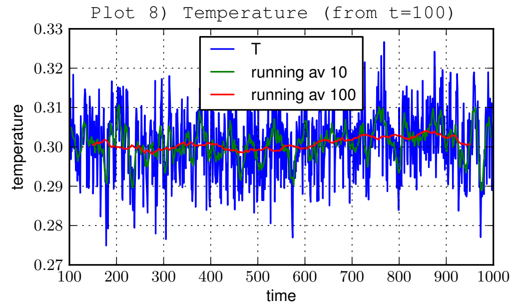


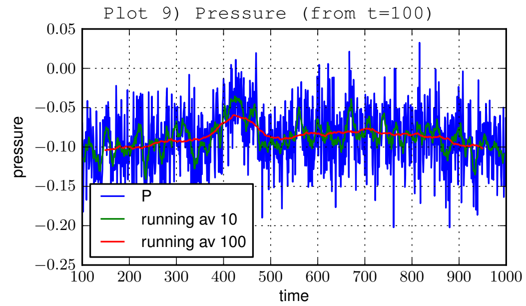


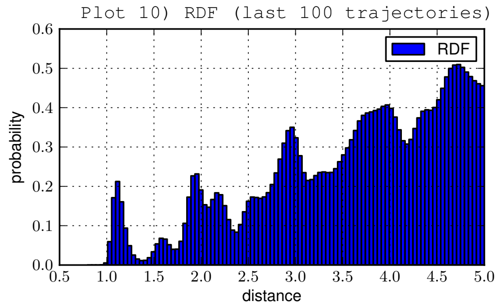




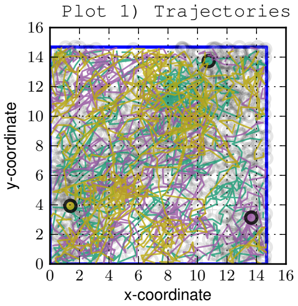


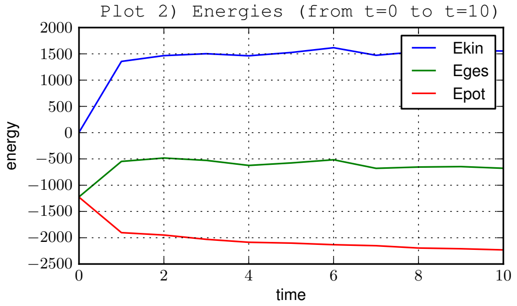


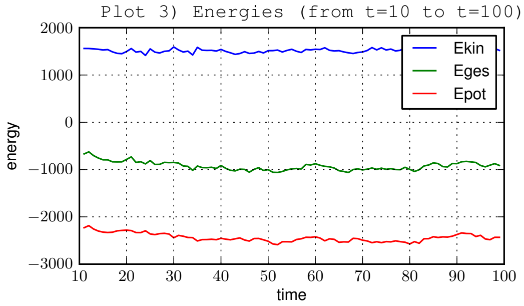


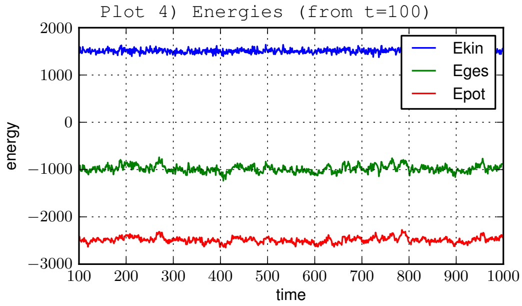


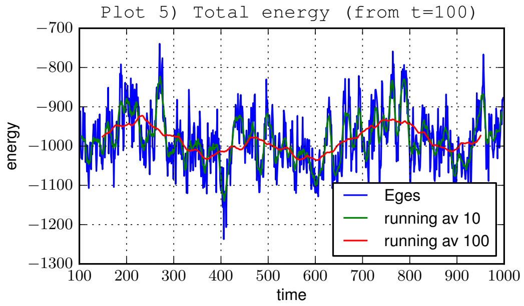
For T=1.0

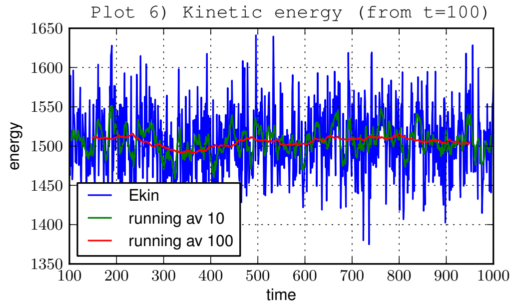

Plot 1) Trajectories
y-coordinate
x-coordinate

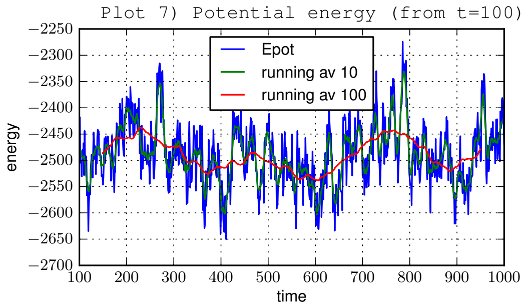

Plot 2) Energies (from t=0 to t=10)
Ekin
Eges
Epot
energy
time

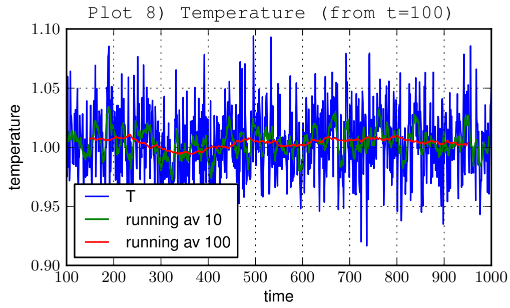

Plot 3) Energies (from t=10 to t=100)
Ekin
Eges
Epot
energy
time

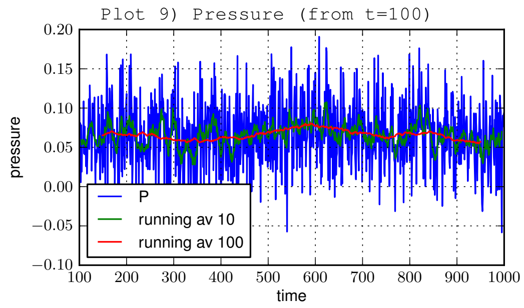

Plot 4) Energies (from t=100)
Ekin
Eges
Epot
energy
time

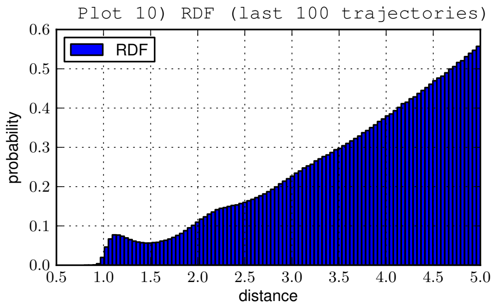

Plot 5) Total energy (from t=100)
Eges
running av 10
running av 100
energy
time


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

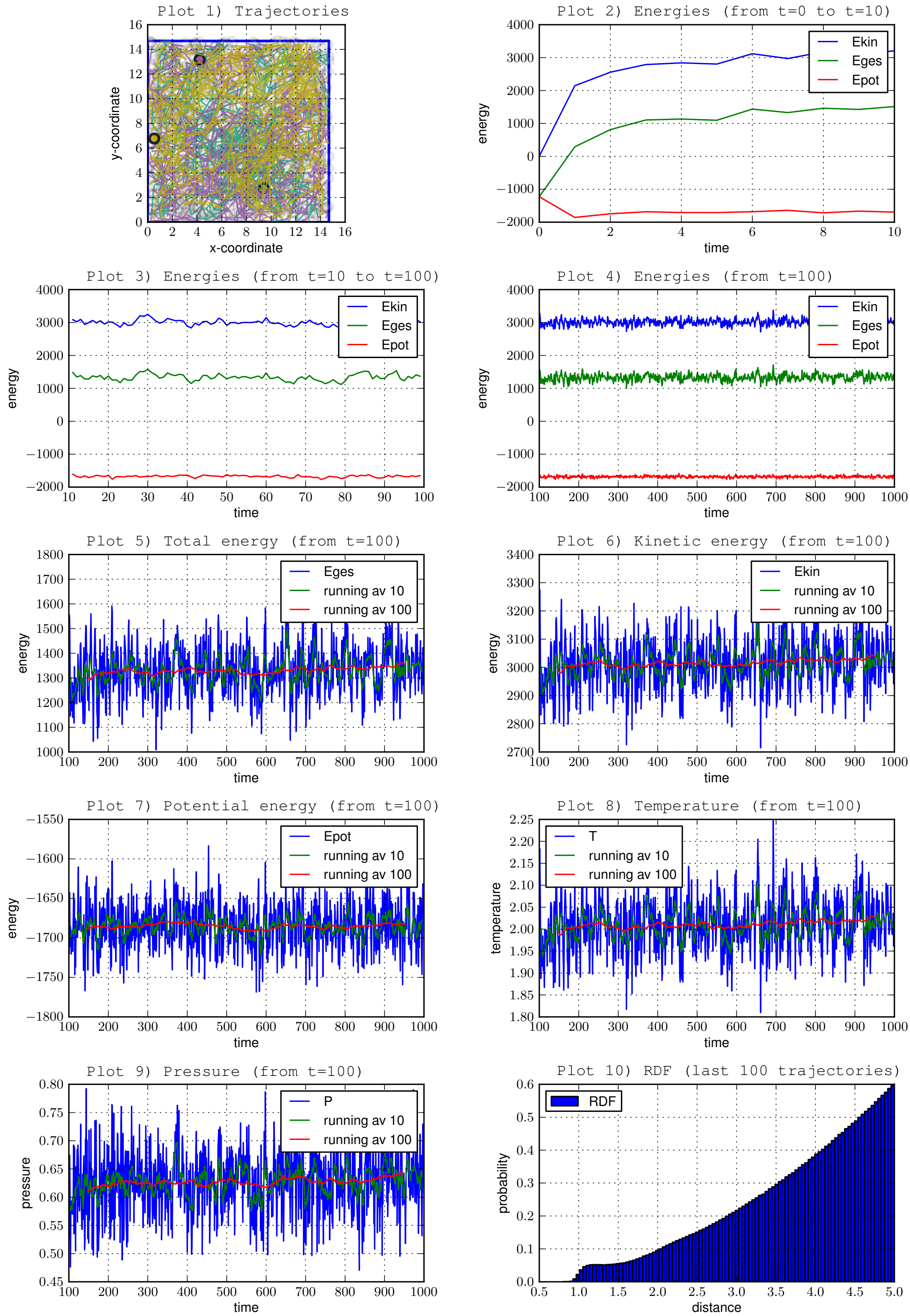

Plot 7) Potential energy (from t=100)
Epot
running av 10
running av 100
energy
time


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


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


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

For T=2.0


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