Particles distribution in both directions parallel or vertical to wall

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1 Theoretical Frame

Considering thousands of colloid particles in fluid, which are interacting with each other through fluid or hydrodynamics interaction, both situations in which we take hydrodynamics interaction into consideration or not will be discussed in this article. They are restricted near a plane close to the wall by harmonic potential. We'll see its distribution in both directions parallel or vertical to the wall with or without hydrodynamics interaction. Some comparison with theory is also included.

We assume that it's Stokes flow(i.e. particle's inertia is ignored) and there's no gravity (i.e. counteracted with buoyancy).

1.1 Direction parallel to the wall

We'll look into particles' distribution along directions parallel to the wall. Particles are initialized as a gaussian distribution right on the plane at the distance of H with the wall.

With Hydrodynamics interaction

Theoretically, when there's HI(Hydrodynamics Interaction), particles that are initialized with Gaussion Distribution would not last as gaussion distribution since there's interaction through dynamics interaction or fluid.

Without Hydrodynamics interaction

Particles would last as gaussion distribution without HI as theory tells us.

The parallel and perpendicular motion can be separated. Thus, we can get the diffusion coefficient below as a result of law of Stokes-Einstein.

$$v_{//} = \mu_{//} F_{//}$$
$$D_{//} = k_B T \mu_{//}$$

where $\frac{\mu_{//}(h)}{\mu_0} = 1 - \frac{9a}{16h} + \frac{2a^3}{16h^3} - \frac{a^5}{16h^5}$,which is approximation of low order.

Since we already have diffusion efficient now, analytic result of standard variance of gaussion distribution would be:

$$\sigma = \sqrt{2Dt}$$

1.2 Direction vertical to the wall

There's a plane of height H on which energy is minimum and make a 2nd order expansion on the energy function of z, which is normal to the wall. $E = \frac{k(h-H)^2}{2}$

We get the Gibbs distribution(also named Boltzmann Distribution):

$$P(h) \sim exp(-\frac{k(h-H)^2}{2k_BT})$$

in the vertical direction with the wall.

2 Simulation

First, we set:
Number of particles: n=4096;
Radius of particle: a=0.656;
viscosity: eta=1.0e-3;
k_BT=0.01656778564
Initial condition
All particles are gaussion distribution on the balance plane(i.e. z=H=5.0). Initial $\sigma 0$ is given as following.
How to set the initial distribution of particles.
Since it is gaussion, we should only make sure of one parameter: $\sigma 0$.
Define packing fraction as $\phi = \pi a^2 n_0 \sim 1$,where a is radius of particles.
Since n satisfies gaussion distribution:

$$n(r, t = 0) = n_0 e^{-r^2/2\sigma_0^2}$$

So: $n_0 = \frac{N}{\int_0^\infty e^{-r^2/2\sigma_0^2} 2\pi r dr} = \frac{N}{2\pi\sigma_0^2}$

Since $\phi \sim 1$, $\sigma 0 = \sqrt{N/2}a$

'initial.m' will be automatically run by 'err_bar_main.m' to get the initial file './data/initial.dat'.

How to set stiffness k

To set k, we should firstly set H, which should be about $5 \sim 10$ times a since they're closed to the wall. We set H=5 in the beginning of this article. Since $H \sim (5 \sim 10)\sigma$ empirically and $\sigma^2 = \frac{k_BT}{k}$, we choose 2 different k as comparison and we'll see some interesting phenomenon with it.

Set $k_BT = 0.0165677856$ and we choose $k = k_BT$ or $4k_BT$ and H is correspondingly 5 or 10 times σ.

How to set iteration time step: dt

There's a trade-off between calculation and accuracy and effectiveness. When dt is too small, calculation would be too time-wasted. However, when dt is too big, data would be oscillatory and inconsistent with reality.

We define relaxation time τ first:

To set a particle at a distance of 0.1H with balance plane. According to its dynamics ODE:

$$\frac{dZ(t)}{dt} = -\mu k(h - H)$$

, where $\mu = \frac{1}{6\pi a\eta}$ is mobility.

We can get its equation of motion:

$$H - Z(t) = 0.1Hexp(-t/\tau)$$

Here $\tau = \frac{6\pi a\eta}{k}$ is relaxation time defined above.

dt is $0.1 \sim 0.25\tau$ empirically and we set dt=0.08 when k=k_BT and dt=0.02 when k=4k_BT to satisfy this rule.

A matlab script 'err_bar_main.m' is written to run simulations for 'repeat' times. And the error bar figure will be output to '/fig/vertical' and '/fig/hori'.

Simultaneously, probability distribution would be recorded into 'data.mat' in current directory.

When plotting figures, standard variance in both directions would be recorded simultaneously as 'sigma_hori' and 'sigma_vertical '.

2.1 Without hydrodynamics interaction

To set 'hydro_interaction=0', we get the situation where hydrodynamics interaction would not be taken into consideration.

2.1.1 k=k_BT

We repeats for 50 times (i.e. repeat=50).

Besides, we run for 200 time steps at each run and output result every 20 time steps.(i.e n_steps=200, n_save=20). Since $\tau = 0.7463$, we set $dt = 0.08$, which is about 0.1τ, and time length is $dt \cdot n\_steps = 16$, which is about 20τ.

The other parameters are set as below:

steps sampling parallel to the wall:r_num_hori=20;

steps sampling vertical to the wall: r_num_vert=10;

step interval parallel to the wall: r_step_hori=3

step interval vertical to the wall: r_step_vert=0.2;

Besides: tau= 0.7463

Finally, the error bar figure in the vertical direction is acquired as fig. 1. It has been taken the logarithmic function such that it would be a straight line if it is a gaussian distribution. The regression is done in both side of the plane.(i.e. left side is below the plane and right side is above the plane.) The estimated line is acquired by computing covariance matrix on all the particles' location.

Here, we only show 3 figures in time sequence and the others are saved by me in case when it's needed.

And the error bar figure parallel to the wall is fig. 2.

As figures show, the simulation results are consist with estimated and analysis cases.The analytic $\sigma = 1$

Moreover, σ vs t is plotted as fig. 3. Notice that scale of vertical coordinate is amplified so that there's difference between σ from simulation and analysis, whose relative error is 0.3% which is much smaller than 10% that we require.

2.1.2 k=$4k_BT$

Since k is 4 times larger, τ is a quarter of original one. Thus, dt, n_steps should be 4 times larger too to make sure that time length is long enough(20τ) and dt is $(0.1 \sim 0.25)\tau$.

Since $\tau = 0.7463/4$, we set $dt = 0.08$, which is about 0.1τ, n_step=800. Thus, time length is $dt \cdot n\_steps = 16$, which is about 80τ and the same with it when k=k_BT.

Parameters are set as below (see their description in front):

repeat=50

dt=0.02;

r_step_vert=0.1;

Besides tau=0.1866, which is 1/4 of it when k=k_BT

Finally, the error bar figure in the vertical direction is acquired as fig. 4. It has been taken the logarithmic function such that it would be a straight line if it is a gaussian distribution.The estimated line is acquired by computing covariance matrix on all the particles' location.

Here, we only show 3 figures in time sequence and the others are saved by me in case when it's needed.

And the error bar figure parallel to the wall is fig. 5.

As figures show, the simulation results are consist with estimated and analysis cases.The analytic $\sigma = 0.5$

Moreover, σ vs t is plotted as fig. 6. Notice that scale of vertical coordinate is amplified so that there's difference between σ from simulation and analysis, whose relative error is 0.3% which is much smaller than 10% that we require.

2.2 With hydrodynamics interaction

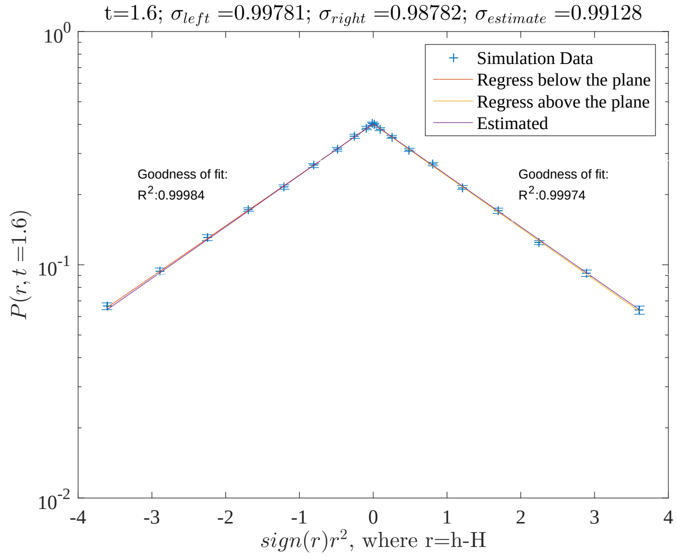
After considering HI, there would be far more interesting phenomenons.

To set 'hydro_interaction=1', we get the situation where hydrodynamics interaction would be taken into consideration.

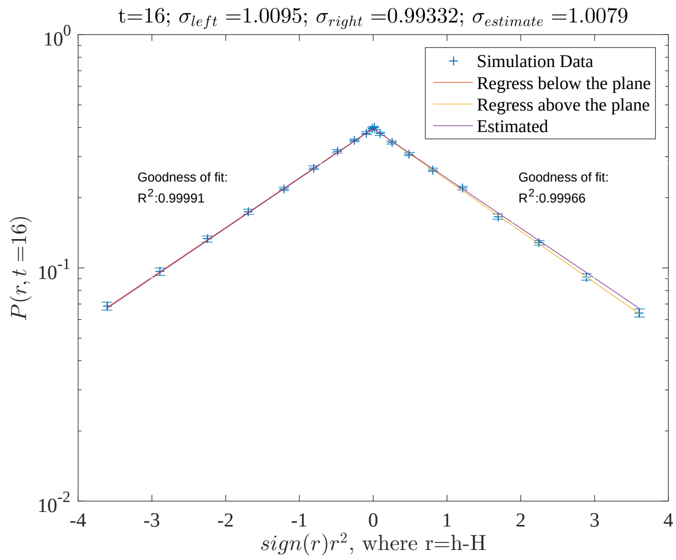
2.2.1 k=k_BT

We repeats for 50 times (i.e. repeat=50).

Figure 1: k=kT,vertical,without HI

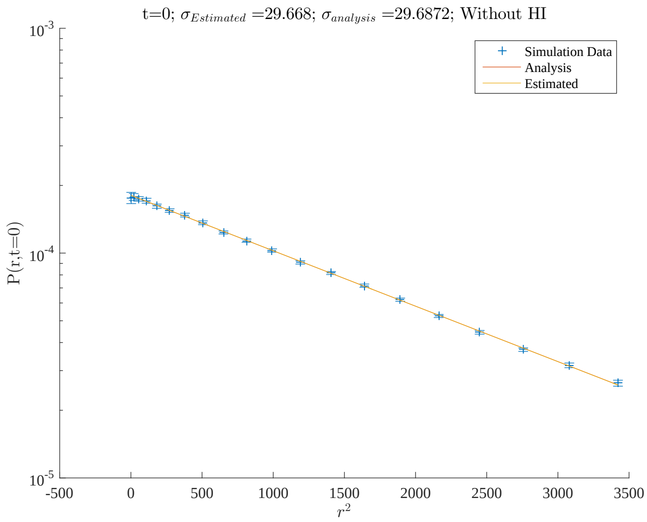


(a) t=1.6

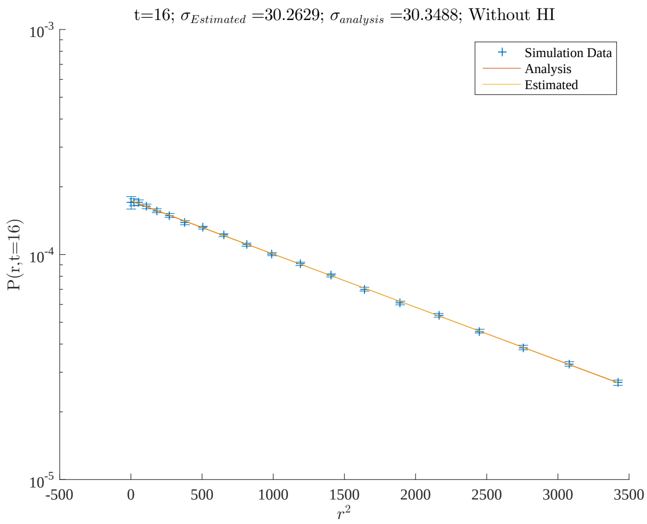


(b) t=16

Figure 2: k=kT,parallel,without HI



(a) t=0



(b) t=16

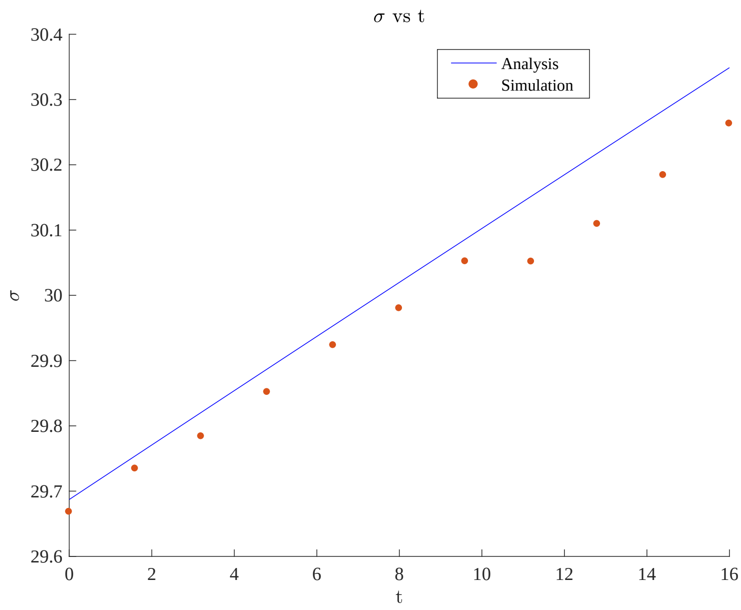


Figure 3: σ vs t, k=kT, parallel, without HI

Besides, we run for 200 time steps at each run and output result every 20 time steps.(i.e n_steps=200, n_save=20). Since $\tau = 0.7463$, we set $dt = 0.08$, which is about 0.1τ, and time length is $dt \cdot n\_steps = 16$, which is about 20τ.

The other parameters are set as below:

steps sampling parallel to the wall:r_num_hori=20;

steps sampling vertical to the wall: r_num_vert=10;

step interval parallel to the wall: r_step_hori=3

step interval vertical to the wall: r_step_vert=0.2;

Besides: tau= 0.7463

Finally, the error bar figure in the vertical direction is acquired as fig. 7.

Here, we only show 3 figures in time sequence and the others are saved by me in case when it's needed.

And the error bar figure parallel to the wall is fig. 8.

As figures show, the simulation results are consist in vertical direction with estimated and analysis cases.The analytic $\sigma_{vertical} = 1$

There's no σ vs t figure since there's no analysis solution when considering HI.

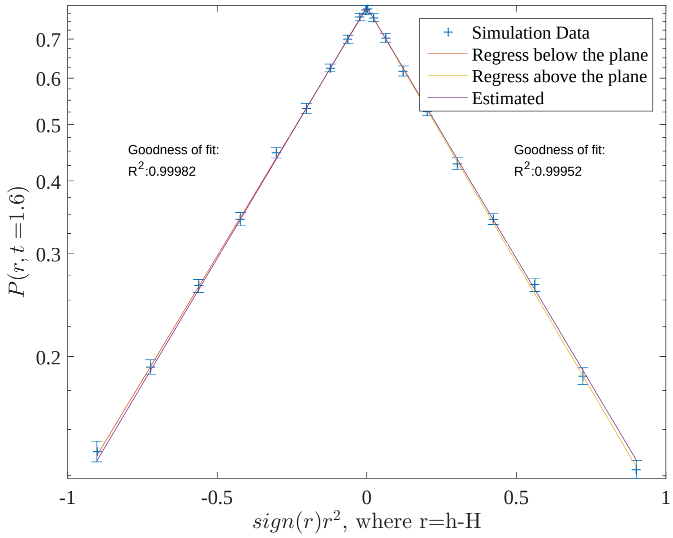
As figures about the parallel direction show, distribution would be more flat as time increase. Notice that the estimated line are gained by covariance matrix of all particles.

Since the logarithm calculation is meaningless here, I also plot the probability distribution (fig. 9)

To see whether it satisfies gaussian distribution when r is large, we enlarge

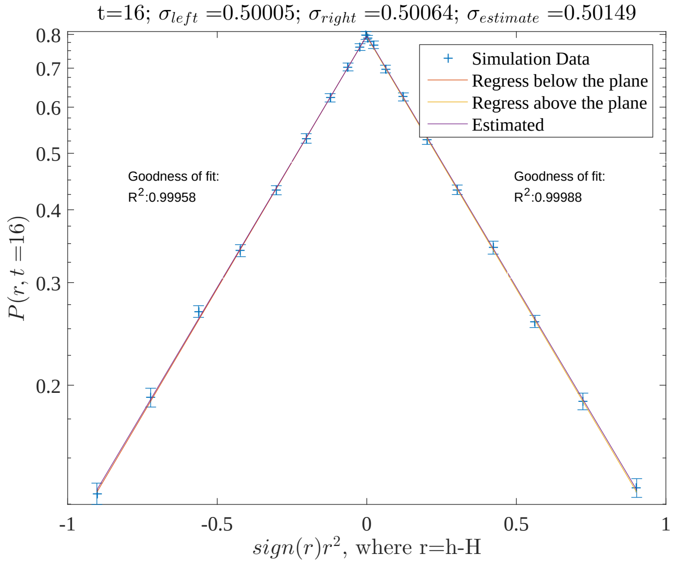
Figure 4: k=4kT,vertical,without HI

t=1.6; σ_{left} =0.50546; σ_{right} =0.49849; $\sigma_{estimate}$ =0.50201



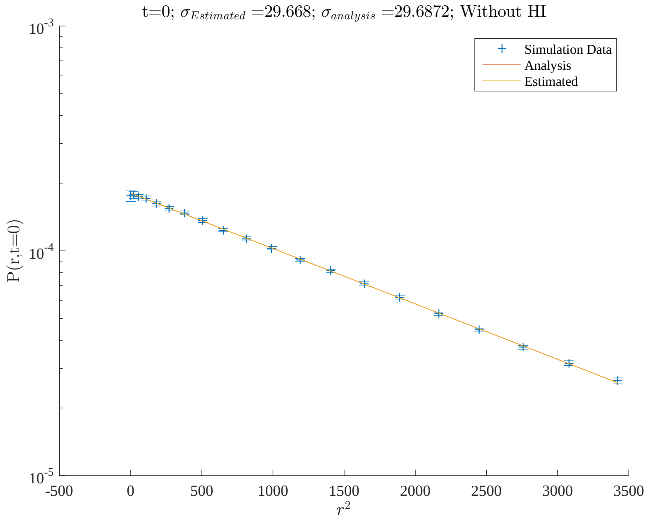
(a) t=1.6

t=16; σ_{left} =0.50005; σ_{right} =0.50064; $\sigma_{estimate}$ =0.50149

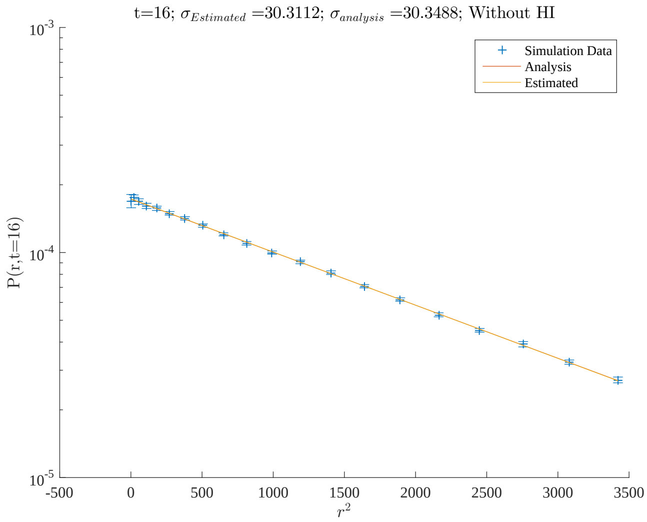


(b) t=16

Figure 5: k=4kT,parallel,without HI



(a) t=0



(b) t=16

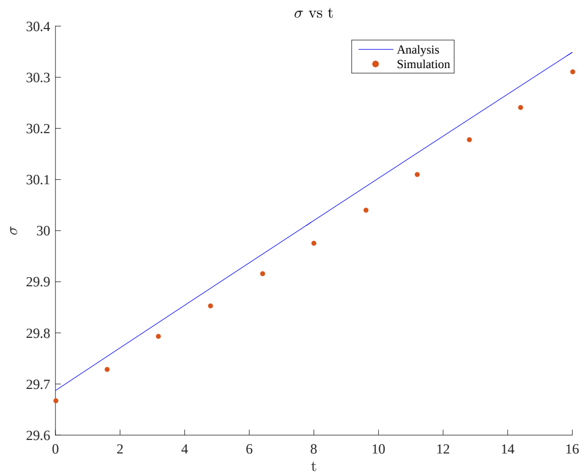


Figure 6: σ vs t, k=4kT, parallel, without HI

r_step_hori to be 10 such that length of r is $20 \times 10 = 200$. Figures with or without logarithm at t=16 are showed in fig. 10

2.2.2 k=$4k_BT$

Since k is 4 times larger, τ is a quarter of original one. Thus, dt, n_steps should be 4 times larger too to make sure that time length is long enough(20τ) and dt is $(0.1 \sim 0.25)\tau$.

Since $\tau = 0.7463/4$, we set $dt = 0.08$, which is about 0.1τ, n_step=800. Thus, time length is $dt \cdot n\_steps = 16$, which is about 80τ and the same with it when k=k_BT.

Parameters are set as below (see their description in front):

repeat=25 (Since time length is 4 times larger and HI is taken into consideration, 50 repeats won't be affordable)

dt=0.02;

r_step_vert=0.1;

Besides tau=0.1866, which is 1/4 of it when k=k_BT

Finally, the error bar figure in the vertical direction is acquired as fig. 11.

Here, we only show 3 figures in time sequence and the others are saved by me in case when it's needed.

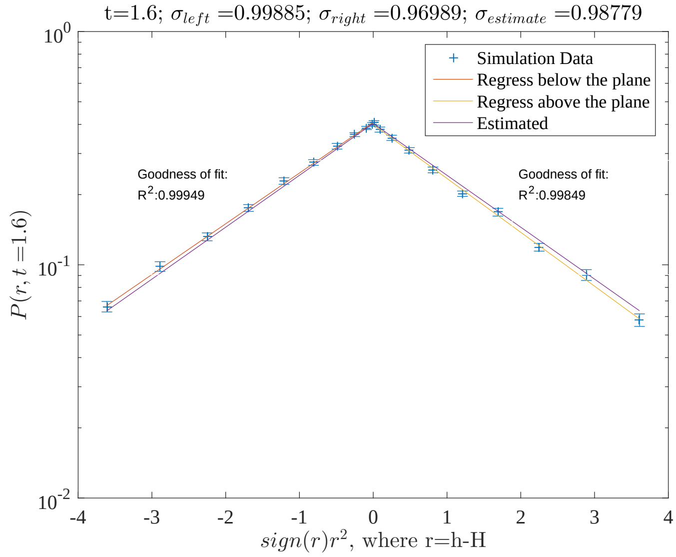
And the error bar figure parallel to the wall is fig. 12.

As figures show, the simulation results are consist in vertical direction with estimated and analysis cases.The analytic $\sigma_{vertical} = 0.5$

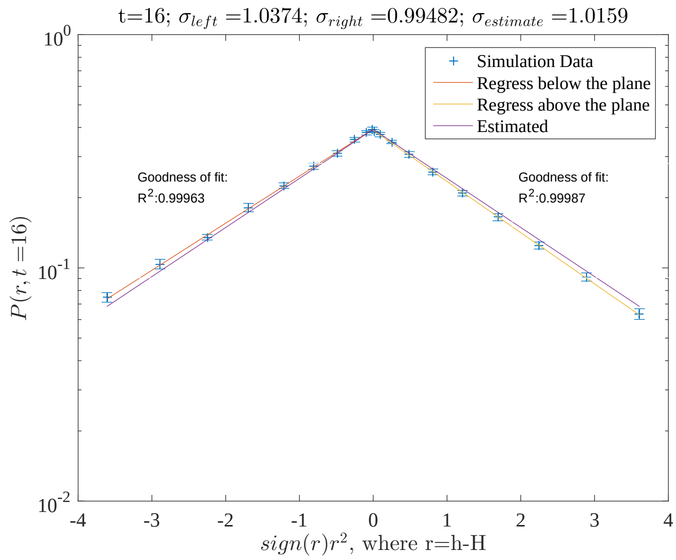
There's no σ vs t figure since there's no analysis solution when considering HI.

As figures about the parallel direction show, distribution would be more flat as time increase. Notice that the estimated line are gained by covariance matrix of all particles.

Figure 7: k=kT,vertical,with HI

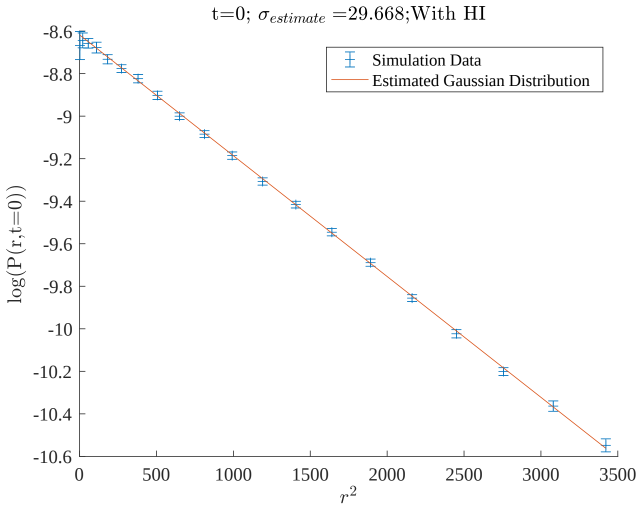


(a) t=1.6

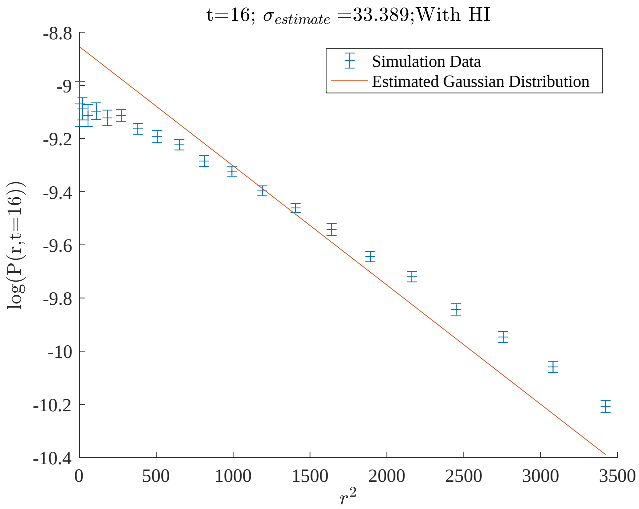


(b) t=16

Figure 8: k=kT,parallel,with HI

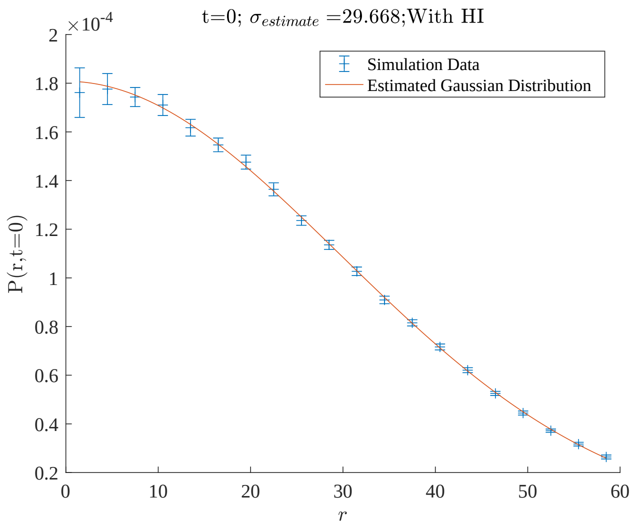


(a) t=0

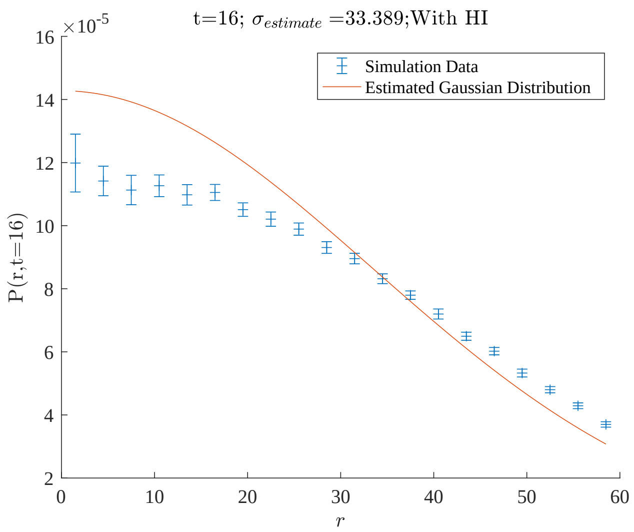


(b) t=16

Figure 9: k=kT,parallel,with HI

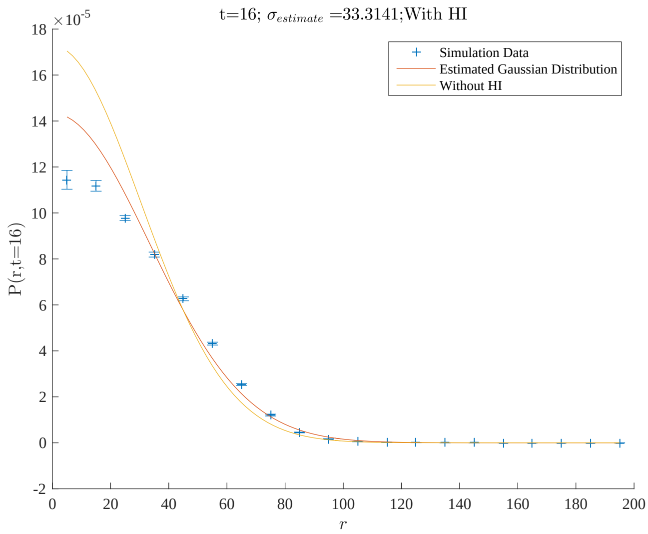


(a) t=0

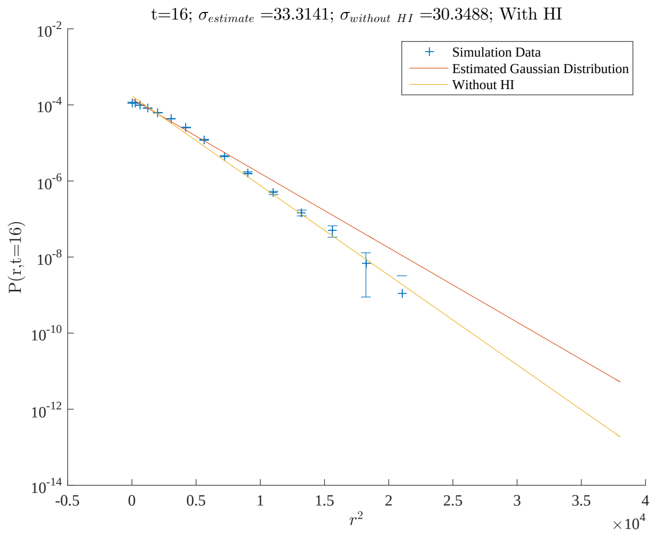


(b) t=16

Figure 10: k=kT,parallel,with HI

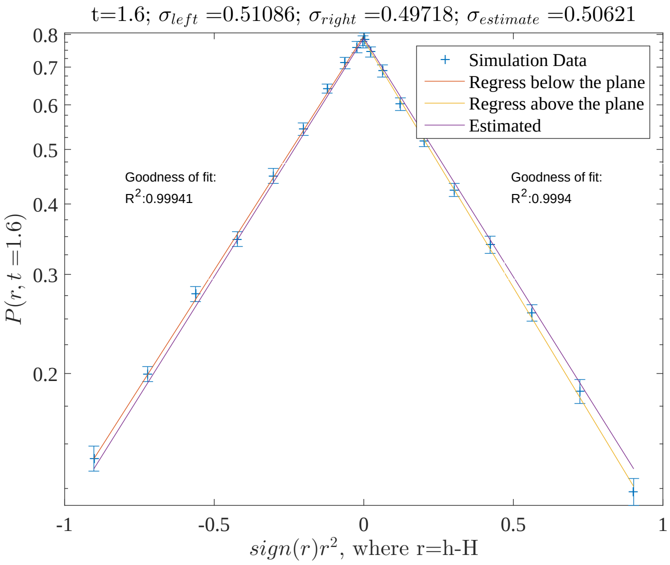


(a) Without log

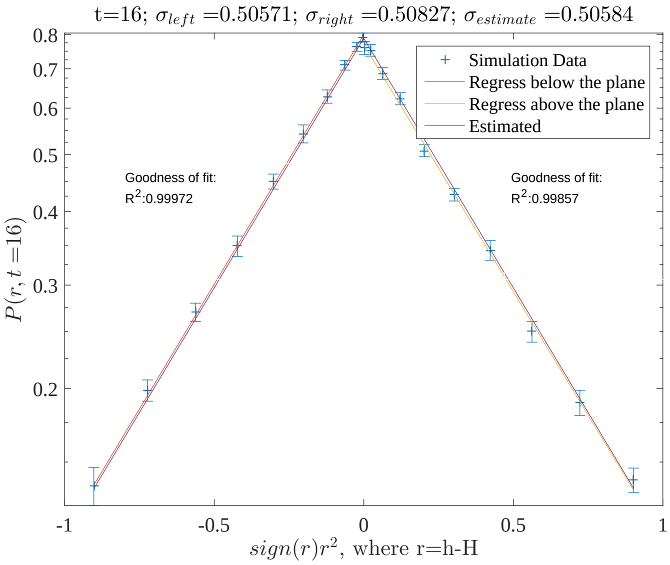


(b) With log

Figure 11: k=4kT,vertical,with HI

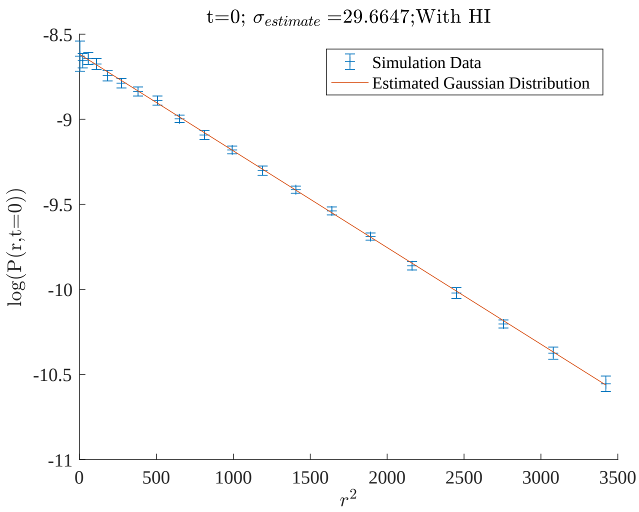


(a) t=1.6

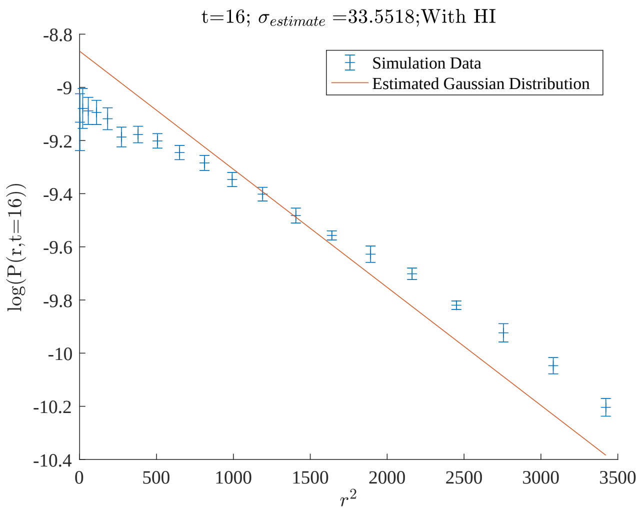


(b) t=16

Figure 12: k=4kT,parallel,with HI



(a) t=0

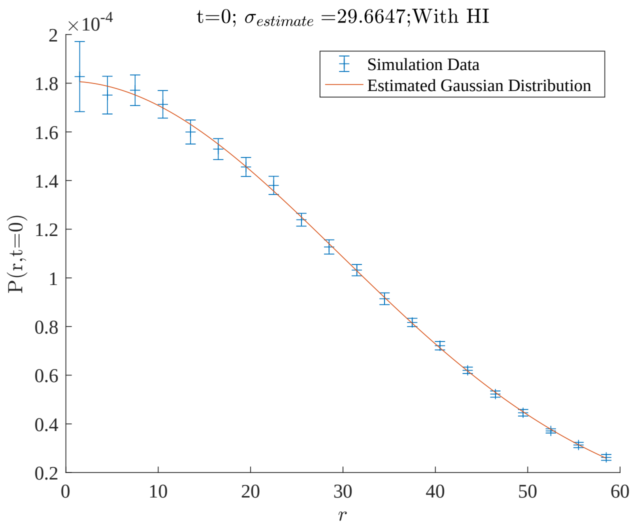


(b) t=16

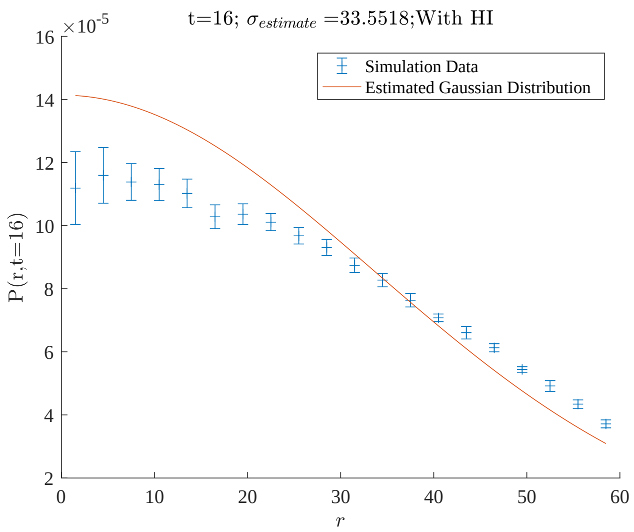
Since the logarithm calculation is meaning less here, I also plot the probability distribution (fig. 13)

Also, to see whether it satisfies gaussian distribution when r is large, we enlarge r_step_hori to be 10 such that length of r is $20 \times 10 = 200$. Figures with or without logarithm at t=16 are showed in fig. 14

Figure 13: k=4kT,parallel,with HI

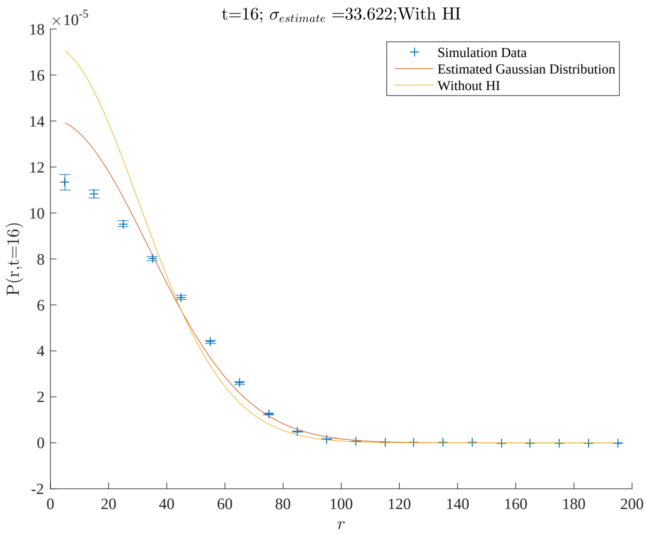


(a) t=0

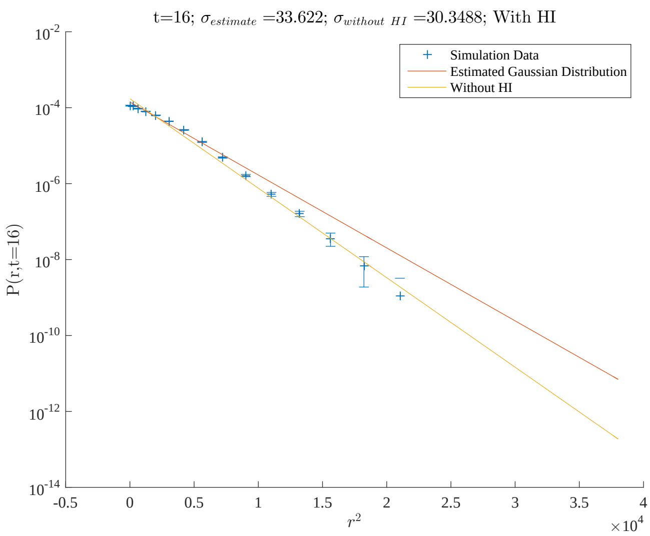


(b) t=16

Figure 14: k=4kT,parallel,with HI



(a) Without log



(b) With log