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Dipartimento di Fisica e Astronomia
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Collective dynamics of active particles

Relatore:
Dott. Beatrice Fraboni

Correlatore:
Dott. Nuno Araujo

Presentata da:
Andrea Angeletti

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Abstract [ITA]

Il nostro scopo è lo studio e il confronto della dinamica di particelle passive e attive in un fluido. Vengono inoltre introdotti i modelli matematici che permettono di simulare il loro comportamento. Sono studiate le propietà e la soluzione numerica dell'equazione di Langevin nella sua approsimazione in regime 'overdamped'. Mostriamo come lo spostamento quadratico medio delle particelle passive sia diffusivo, *i.e.* lineare nel tempo, e proporzionale al coefficiente di diffusione lineare, mentre quello di particelle attive quadratico per un tempo minore dell'inverso del coefficiente di diffusione rotazionale e diffusivo per un tempo maggiore. Con la presenza di una parete repulsiva e osservando la distribuzione di probabilità della posizione delle particelle, notiamo come quelle attive tendano ad accumularsi su di essa. Infine osserviamo che sotto l'azione di un potenziale repulsivo particelle attive tendono a formare agglomerati.

Abstract [ENG]

Our aim is to study the collective dynamics of active and passive particles in a fluid and to give an introduction to the mathematical *methods* and models to simulate their behaviour. We study the physical property and numerical solutions of the Langevin equation in overdamped regime. We show that the mean square displacement of passive particles scales (asymptotically) in time and the slope is proportional to a constant term, the Diffusion coefficient. We compare it to the one of active particles which undergoes a ballistic regime, quadratic in time, for a time shorter than the inverse of the diffusion rotational coefficient and becomes diffusive for a longer time. Under the presence of planar repulsive boundary, like a wall, active particles tend so accumalate on it. Under a repulsive force between them, active particles tend to form cluster.

Contents

Chapter 1

Introduction

In this work we study and simulate the collective properties of a large system of N particles in a fluid.

This work has been realized in Portugal during an Erasmus exchange period. A special thanks goes to Nuno Araujo of the University of Lisbon. I am very grateful to him for introducing me to this interesting topic and for the help he gave me during the developoment process of the thesis. He was deeply involved in the entire project and his advices and editing work made this work complete.

We model the particles as rigid spheres with a radius $R = 1$ μm and the fluid a liquid at temperature $T = 300$ K, in thermodynamic equilibrium and of a viscosity $\eta = 0.001$ Ns/m^2 [1]. Under these conditions for the value of the diffusion coefficient D_t and of the rotational diffusion coefficient D_r we have $D_t \approx 0.22$ μm$^2 s^{-1}$ and $D_r \approx 0.16$ rad$^2 s^{-1}$, where

$$D_t = \frac{k_B T}{\gamma} \text{ and } D_r \equiv \tau_r^{-1} = \frac{K_b T}{8\pi\eta R^3}$$

and k_B is the Boltzmann costant , $\gamma = 6\pi\eta R$ the Stoke coefficient. The meaning of these coefficients will be explained later. All the values just given are the ones used to perform the simulations, unless stated otherwise.

Before we go deeper into the subject note that the conditions we settled could truthfully represent for example the situation of a collection of many bacterias immersed in water. For this reason these particles are also called microswimmers. Actually one of the main goal of our study is a better understanding of the collective behaviour of a large collection of active particles of the order of the micrometer. Viceversa the results of our theory can and should be tested with experimental observations of collection like the one we have just described. In fact, nowadays engineers can control the motion of particles of the size of the micrometer. This opens the way to several applications. In the case of active particles we can use their ability of self-propelling and thus drive themselves out

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[1]Actually this is the viscosity of water at a temperature of 300 K. Source https://wiki.anton-paar.com/en/water/

of equilibrium. An important example is the possibility to control the motion of artificial or natural microswimmers and use them to carry specific substances to some parts of our body.

The surrounding medium where the particles are immersed, is made up of molecules, much smaller than the particles, that move randomly because of their thermal agitation and collide with the particles,(and among themselves). These collisions generate a net force on the particles. We cannot consider all the single interactions neither solve all the equations of motion of all the molecules. It would require to solve a number of equations of the order of the Avogado number which could require huge computational power. Instead of it, we assume that the dynamics of each particle is described by the Langevin equation where the force experienced by a particle is represented by a stochastic term $A\vec{\xi}$. A has the dimensions of a force and $\vec{\xi}$ is a 3-dimensional vector with the following property:

$$\left\langle \xi_i(t) \right\rangle = 0 \tag{1.1}$$

$$\left\langle \xi_i(t_1)\xi_j(t_2) \right\rangle = \delta_{ij}\delta(t_1 - t_2) \tag{1.2}$$

with $i = 1, 2, 3$. The $\left\langle \right\rangle$ operator represents the average overall al the particles.

Equation (1.1) means that the mean value of ξ_i over time is zero. This states that the interactions between the fluid and the particles have no preferential direction.

Equation (1.2) means that the values assumed by the component of $\vec{\xi}(t)$ are uncorrelated in space and time.

We assume also that $\xi_i(t)$ follows the Gaussian distribution. Thus by (1.1) and (1.2) we conclude that mean value of $\xi_i(t)$ is zero and its standard deviation is one.

The most important quantity that we can study and that we are going to observe in this work is the mean square displacement, averaged over all the N particles of the system and considered as a function of a time. We label it by $MSD(t)$ and it is given by:

$$MSD(t) = \frac{1}{N}\sum_{k=1}^{N} [\, \vec{x_k}(t) - \vec{x_k}(t_0) \,]^2 \tag{1.3}$$

where

$$[\, \vec{x_k}(t) - \vec{x_k}(t_0) \,]^2 = \sum_{i=1}^{3} [x_i(t) - x_i(t_0)]^2 \tag{1.4}$$

and $\vec{x_k}(t)$ is the position at the time t of k-particle and $\vec{x_k}(t_0)$ its initial position. Thus the $MSD(t)$ is just the average distance traveled from the particles of the system from their initial position.

In each chapter we derive the algorithms which we used in the code and compare the results of the simulation with the theoretical predictions.

In chapter 2 we introduce the Langevin equation and find the numerical value of the A coefficient, which is the magnitude of the random force which origins from the interaction

between the fluid molecules and the particles.

In chapter 3 we focus our attention on passive particles and solve numerically the Langevin equation on the overdamped regime.

In chapter 4 we explain the concept of active particle and model their behaviour by several assumptions.

In chapter 4 we study the effects caused by the presence of boundary, (a planar wall), observing the density probability distribution of the positions, and with attention for the active particles.

In chapter 5 we introduce a pairwise repulsive potential between the active particles and see how this leads them to form cluster.

Chapter 2

Langevin equation

The dynamic of each particle is described by the Langevin equation:

$$m\ddot{\vec{x}}(t) = -\gamma\dot{\vec{x}}(t) + A\vec{\xi}(t) \tag{2.1}$$

The term $-\gamma\dot{x}(t)$ represents the friction force of the fluid.

Equation (2.1) is a set of three equations, one for each translational degree of freedom. Since there is no correlation between the components of the force $A\vec{\xi}$, they are independent. Thus we can study each of them separately. We write indeed:

$$m\ddot{x}_i(t) = \gamma\dot{x}_i(t) + A\xi_i(t) \ . \tag{2.2}$$

If we forget the i-index, we are now looking for a solution of the form :

$$\dot{x}(t) \equiv v(t) = e^{-\frac{\gamma t}{m}}f(t) \tag{2.3}$$

which replaced into equation (2.1) and with $\beta \equiv \frac{\gamma}{m}$ gives:

$$-\beta v(t) + e^{-\beta t}\dot{f}(t) = -\beta v(t) + \frac{A}{m}\xi(t)$$

$$\Leftrightarrow \dot{f}(t) = \frac{A}{m}e^{\beta t}\xi(t)$$

$$\Leftrightarrow f(t) = f(0) + \frac{A}{m}\int_0^t e^{\beta t'}\xi(t')\mathrm{d}t'$$

and so (2.3) becomes:

$$v(t) = f(0)e^{-\beta t} + e^{-\beta t}\frac{A}{m}\int_0^t e^{\beta t'}\xi(t')\mathrm{d}t' \ . \tag{2.4}$$

Evaluating equation (2.4) in $t = 0$ gives:

$$f(0) = v(0)$$

and finally we can write:

$$v(t) = v(0)e^{-\beta t} + e^{-\beta t}\frac{A}{m}\int_0^t e^{\beta t'}\xi(t')\mathrm{d}t' \ . \tag{2.5}$$

By the equation (1.1) we find that:

$$\langle v(t)\rangle = v(0)e^{-\beta t} \ .$$

The average speed of the particles decays exsponentially in a time β^{-1} due to their very small mass m. Note that the $<>$ operator can be moved inside the integral because is it an average overall the particles and does not depend on time.

Squaring and taking the average of the equation (2.5) we get:

$$\langle v_i(t_1)v_j(t_2)\rangle = v_0^2\langle e^{-\beta(t_1+t_2)}\rangle + e^{-\beta(t_1+t_2)}\left(\frac{A}{m}\right)^2\int_0^{t_1}\int_0^{t_2}e^{-(\beta t_1'+t_2')}\langle\xi_i(t_1')\langle\xi_j(t_2')\rangle\mathrm{d}t_1'\mathrm{d}t_2'$$

$$+ v_0\frac{A}{m}e^{-\beta(t_1+t_2)}\left(\int_0^{t_1}e^{-\beta t_1'}\langle\xi_i(t_1')\rangle\mathrm{d}t_1' + \int_0^{t_2}e^{\beta t_2'}\langle\xi_j(t_2')\rangle\mathrm{d}t_2'\right) =$$

where the cross terms vanish. Le us focus now on:

$$\int_0^{t_1}\int_0^{t_2}e^{-(\beta t_1'+t_2')}\langle\xi_i(t_1')\langle\xi_j(t_2')\rangle\mathrm{d}t_1'\mathrm{d}t_2' =$$

$$= \int_0^{t_1}\int_0^{t_2}e^{-(\beta t_1'+t_2')}\delta_{ij}\delta(t_1'-t_2')\mathrm{d}t_1'\mathrm{d}t_2'$$

$$= \int_0^{t_1}e^{-2\beta t_1'}\delta_{ij}\mathrm{d}t_1'$$

Now we can go on and with $i=j$ and $t_1=t_2\equiv t$:

$$\langle v_i^2(t)\rangle = v_0{}^2e^{-2\beta t} + e^{-2\beta t}\left(\frac{A}{m}\right)^2\frac{m}{2\gamma}\left[e^{2\beta t}-1\right]$$

and in the condition when the system reaches the thermodyamic equilibrium:

$$\lim_{t\to\infty}\langle v_i^2(t)\rangle = \frac{A^2}{2m\gamma}$$

$\forall\, i = 1,2,3$ and d the number of spatial dimensions. .

According to the equipartion theorem of thermodynamic we then have:

$$\frac{1}{2}m\langle v^2(t)\rangle = \frac{dk_BT}{2}$$

and since

$$\left\langle v^2(t) \right\rangle = d\left\langle v_i^2(t) \right\rangle$$

we obtain:

$$A = \sqrt{2k_B T \gamma} = \sqrt{2\gamma^2 D_t} \tag{2.6}$$

Chapter 3

Overdamped regime

The overdamped regime is an approximation of the Langevin equation that sets $m\ddot{x} \simeq 0$. Under this condition and substituing the value of A in the Langevin equation (2.1), it becomes:

$$\gamma\dot{\vec{x}}(t) = \sqrt{2\gamma^2 D_t}\,\vec{\xi}(t)$$

Reducing again to one dimension we write:

$$\dot{x}(t) = \sqrt{2D_t}\,\xi(t) \tag{3.1}$$

whose solution is

$$x(t) = x(0) + \sqrt{2D_t}\int_0^t \xi(t')\mathrm{d}t' \tag{3.2}$$

The mean square displacement in one dimension is $MSD(t) \equiv \langle x^2(t) - x(0)\rangle$ and assuming $x(0) = 0$ it is clear:

$$\langle x^2(t)\rangle = \langle 2D_t\int_0^t \xi_i(t')\mathrm{d}t'\int_0^t \xi_i(t'')\mathrm{d}t''\rangle = 2D_t\int_0^t\int_0^t \langle\xi_i(t')\xi_i(t'')\rangle\mathrm{d}t''\mathrm{d}t' =$$

$$2D_t\int_0^t\int_0^t \delta(t_1' - t_2'')\mathrm{d}t'\mathrm{d}t'' = \left(\frac{A}{\gamma}\right)^2\int_0^t \mathrm{d}t' = 2D_t\,t$$

Consequently:

$$\langle\vec{x}^2(t)\rangle = d\langle x_i^2(t)\rangle = 2dD_t\,t \tag{3.3}$$

A careful analysis of equation (3.2) tell us that the position of a particle at the time $t_0 + \Delta t$ will differ from the one at the time t_0 by a term due to the overall effect of the forces acting on it during the interval Δt. This term is the sum of all the contributes of the forces pushing the particle to the left and to the right during the Δt interval time. We now call this term:

$$\sqrt{2D_t}\int_{t_0}^{t_0+\Delta t} \xi(t)\mathrm{d}t \equiv \eta(t_0)$$

and write equation (3.2) as:

$$x(t_0 + \Delta t) = x(t_0) + \eta(t_0)$$

Let us find the properties of $\eta(t)$:

$$\langle \eta(t_0) \rangle = \sqrt{2D_t} \int_{t_0}^{t_0 + \Delta t} \langle \xi(t) \rangle \mathrm{d}t = 0$$

.

$$\langle \eta_i(t_1)\eta_j(t_2) \rangle = 2D_t \int_{t_1}^{t_1 + \Delta t} \int_{t_2}^{t_2 + \Delta t} \langle \xi_i(t_1')\xi_j(t_2') \rangle \mathrm{d}t_1' \mathrm{d}t_2' =$$

$$= 2D_t \int_{t_1}^{t_1 + \Delta t} \int_{t_2}^{t_2 + \Delta t} \delta_{ij}\delta(t_1' - t_2')\mathrm{d}t_1'\mathrm{d}t_2' = 2D_t\delta_{ij}\Delta t$$

We conclude that $\eta(t)$ obeys to the Gaussian distribution and it has a mean value equal to zero and and variance equals to $\sqrt{2D_t\Delta t}$. In practice we use a random number generator, (one for each translational degree of freedom), and with a Gaussian distribution. The mean is zero and a unitary standard deviation which we then multiply by $\sqrt{2D_t\Delta t}$.
Thus in our simulation we compute the position of the particle at discrete time steps where the position of each particle is given by the following algorithm:

$$x(t_0 + \Delta t) = x(t_0) + \sqrt{2D_t\Delta t}\, \xi(t_0 + \Delta t) \tag{3.4}$$

It is come the time to have a look on the result of figure (3.1). It is important to say that in this simulation all the particles have the same initial position, equal to zero, and they are free to expand everywhere with any boundary conditions. The fit made on the simulated points, gave us a value of D_t roughly equal to 0.22 $\mu m^2 s^{-1}$ which is what we expected. The uncertainty is not reported because was too small.
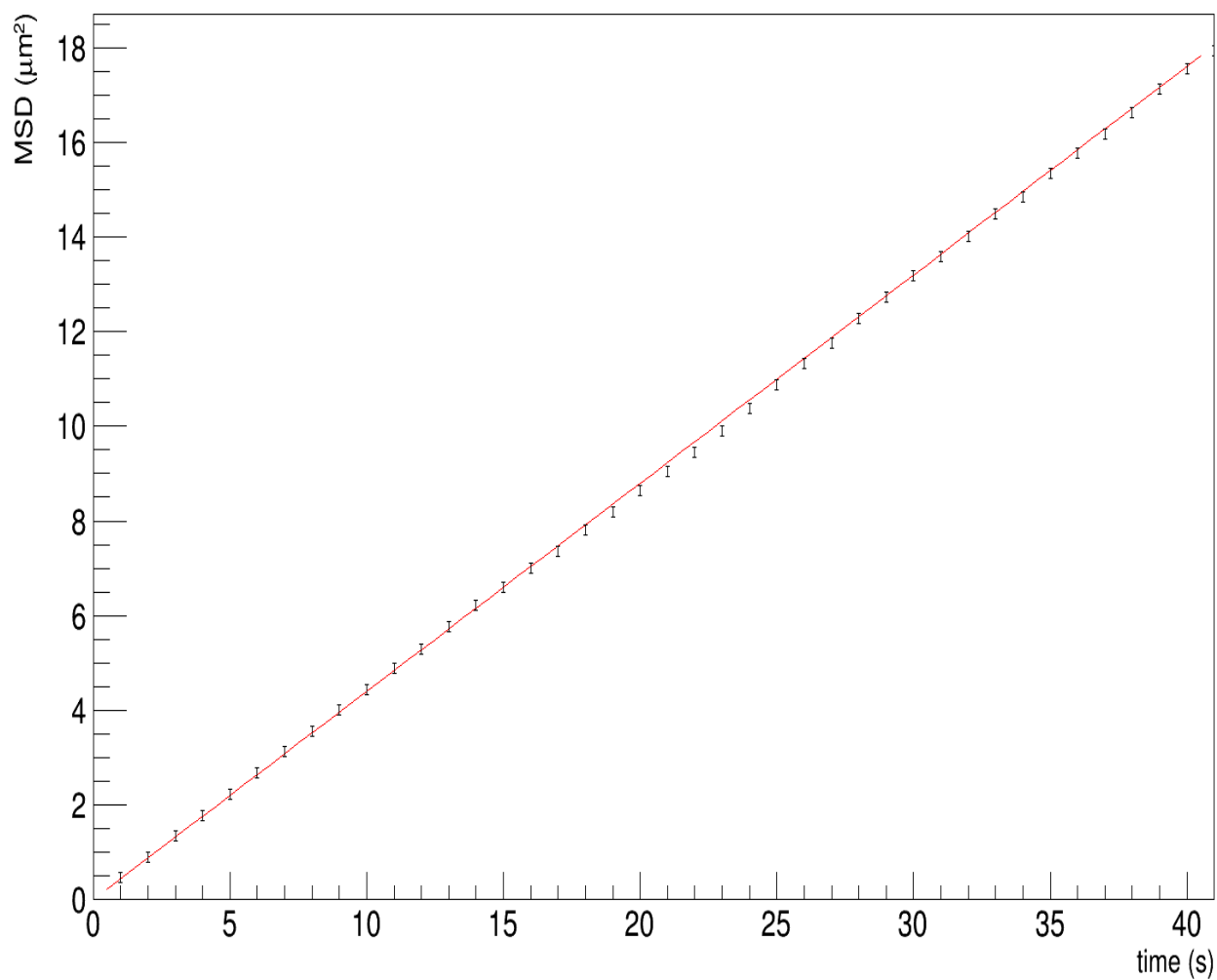
Figure (3.1)   Mean square displacement of passive particles in one dimension.
The red line is the theoretical value. The black points with the error barrs are the result
of the simulation.
The used parameters to run the simulation are $\Delta t = 10^-4$ and $N = 10^3$.

Chapter 4

Active particles

Active matter systems are able to take energy from their environment and drive themselves far from equilibrium (Ramaswamy, 2010). In this chapter we are going to study the mean square displacement of active particles in two dimensions. In our work we refer to active particle as a particle that is characterized by a intrinsec velocity vector $\vec{v}$ and that moves at costant speed v. In nature are observed some micro-swimmer with similar property. An example are the spermatozoon. Their motion is not random but has a preferred direction of velocity. We call this velocity the drift velocity $\vec{v}$. (Ramaswamy, 2010)

We performed our simulatiom reproducing the behaviour of active particles in *two dimensions* and we made several assumptions:

- $\vec{v}(t) = v \left(\cos(\varphi(t)) \, \hat{i} \, , \, \sin(\varphi(t)) \, \hat{j} \, \right)$;

- the magnitude v of the drif velocity $\vec{v}$ is the same for all the particles of the system;

- φ sweeps $360°$ in a time equal to τ_r ;

- φ satisfies:

$$\dot{\varphi}(t) = B_\varphi \xi_\varphi(t) \tag{4.1}$$

  where B_φ is a dimensionless costant and ξ_φ has the same properties of ξ_i. As we did with equation (3.1) we conclude that:

$$\left\langle \varphi(t)^2 \right\rangle \sim 2D_r t$$

In the introduction we talked about τ_r, now we are able to grasp its meaning. It represents the time that an active particle take to make an entire rotation over itself. The higher is τ_r the faster tha particle loses the initial information about its initial preferential direction and so its motions becomes more and more random.

We can finally write down the equations of motions:

$$\dot{x}(t) = \sqrt{2D_t} \, \xi_x(t) + v \cos \varphi(t) \tag{4.2}$$

$$\dot{y}(t) = \sqrt{2D_t}\,\xi_y(t) + v\sin\varphi(t) \tag{4.3}$$

It can be showed that the mean square displacement $MSD(t)$ of active particles in two dimension, is given by [1] :

$$MSD(t) = (4D_t + 2v^2\tau_r)t + 2v^2\tau_r^2(e^{-t/\tau_r} - 1) \tag{4.4}$$

We are not going to verify this result numerically.
In the limit $t \gg \tau_r$ of equation (4.4) we have that :

$$MSD(t) \propto (4D_t + 2v^2\tau_r)t \tag{4.5}$$

and recalling equation (3.3) we conclude that the $MSD(t)$ of active particles becomes diffusive with an effective diffusion coefficient given by

$$D_{eff} = D_t + \frac{1}{2}v^2\tau_r \tag{4.6}$$

Thus by equation (4.6) the theorical value of the effective diffusion coefficient is $D_{eff} \simeq 3.35\mu\mathrm{m}^2 s^{-1}$.
We are going to see that the $MSD(t)$ underogoes a ballistic regime in time much smaller then order of τ_r and shows a transition to the diffusive behaviour.
It worth to note here that $\tau_r \simeq 6.3\ s$.
Now we would like to know the algorithm to perform our simulation. Let us start.
In this situation we need to know how the $\varphi(t)$ angle evolves. We can easily find :

$$\langle\varphi(t)^2\rangle = B_\varphi \int_0^t \int_0^t \langle\xi_\varphi(t')\xi_\varphi(t'')\rangle \mathrm{d}t''\mathrm{d}t' = B_\varphi$$

$$\Rightarrow B_\varphi = \sqrt{2D_r}$$

and finally say

$$\varphi(t_0 + \Delta t) = \varphi(t_0) + \sqrt{2D_r\Delta t} \tag{4.7}$$

Thus in our code what we really use, as we saw before in chapter 3, is a random number generator with a Gaussian distribution, zero mean and unitary standard deviation which we then multiply by $\sqrt{2D_r\Delta t}$.

The solution of equation (4.2) is

$$x(t_0 + \Delta t) = x(t_0) + \int_{t_0}^{t_0+\Delta t} \left(\sqrt{2D_t}\xi_x(t) + v\cos\varphi(t)\right)\mathrm{d}t$$

We have already worked out the part of the integral containing the $\sqrt{2D_t}\xi_x(t)$ term, see equation (3.4). In the approximation that the angle $\varphi(t)$ remains costant during the Δt interval we easily find the algorithm to simulate the x-position of a particle:

$$x(t_0 + \Delta t) = x(t_0) + \sqrt{2D_t\Delta t}\, \xi_x(t_0 + \Delta t) + v\cos\varphi(t_0 + \Delta t)\Delta t$$

In the same way:

$$y(t_0 + \Delta t) = y(t_0\Delta t) + \sqrt{2D_t\Delta t}\, \xi_y(t_0 + \Delta t) + v\sin\varphi(t_0 + \Delta t)\Delta t$$

Let's have a look to our results.

In this chapter, as we did for passive particles, in both simulations all the particles have the same initial position equal to zero and they are free to move everywhere with any boundary conditions. The initial angle φ was uniformly distribuited between $[0:2\pi]$.

Figure (4.1) shows the $MSD(t)$ for one value of the drift velocity, $v = 1\ \mu ms^{-1}$. In the graph are depicted all the values of the $MSD(t)$ in order to make evident its initial behaviour. The experimental value of D_{eff} is roughly $3.35\ \mu m^2 s^{-1}$, in agreement with the theoretical value. The uncertainty is not reported because it was too small. It is interisting to note that the fit was made starting from twenty seconds, which is not too big compared with the value of τ_r which is about six seconds. It suggests that the transition between the two regime is quite fast and clear, as also showed in the plot.

In figure (4.2) are represented the plots of the $MSD(t)$ for four different values of drift velocity (inclunding the case of passive particles).
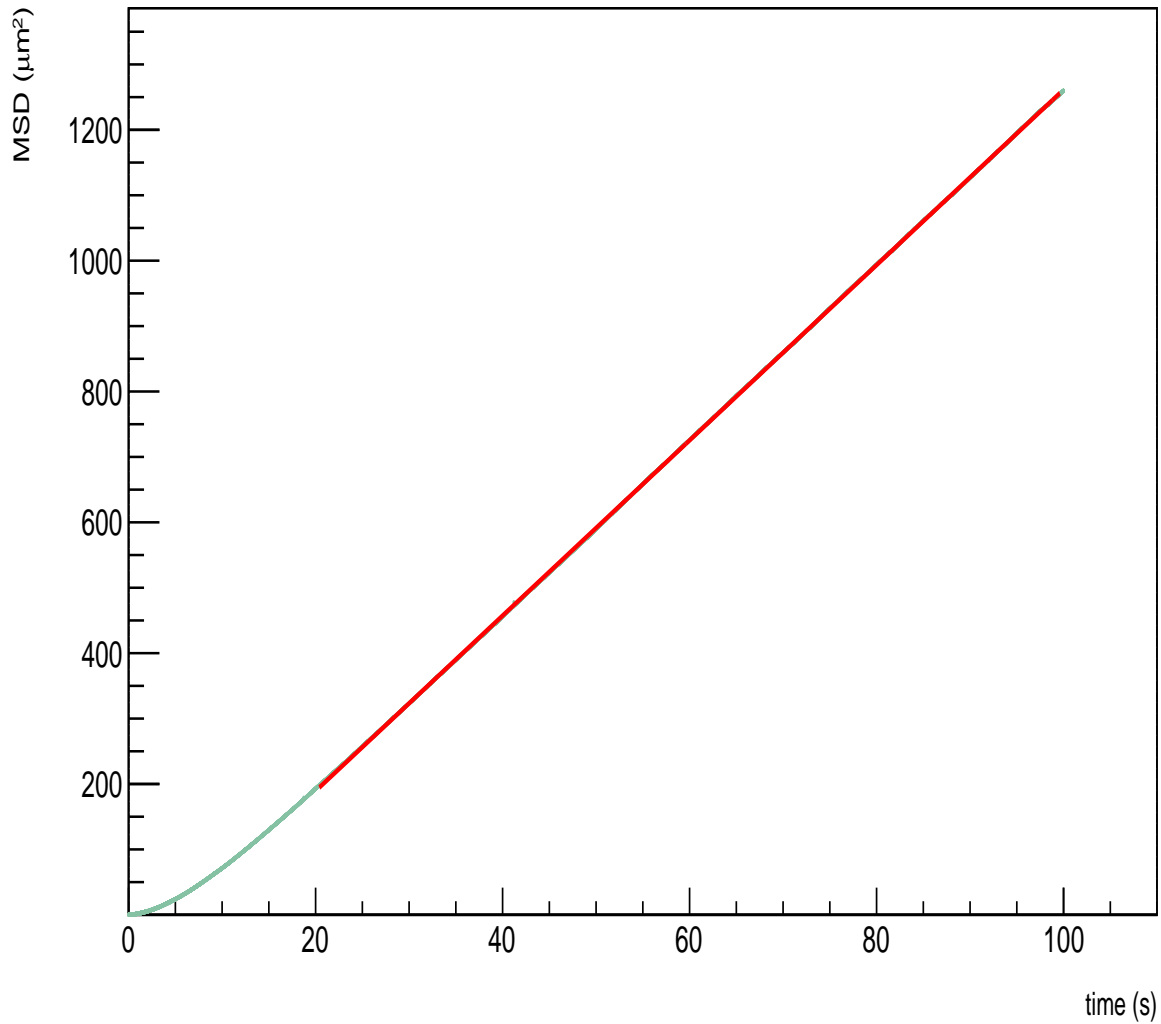
Figure (4.1)   Mean square displacement of active particles in two dimensions.
We can see how the $MSD(t)$ goes from a ballistic regime , approximately quadratic in time and then becomes diffusive , linear in time. The transition between the two regime happens in narrow range between 5 seconds and 10 seconds.
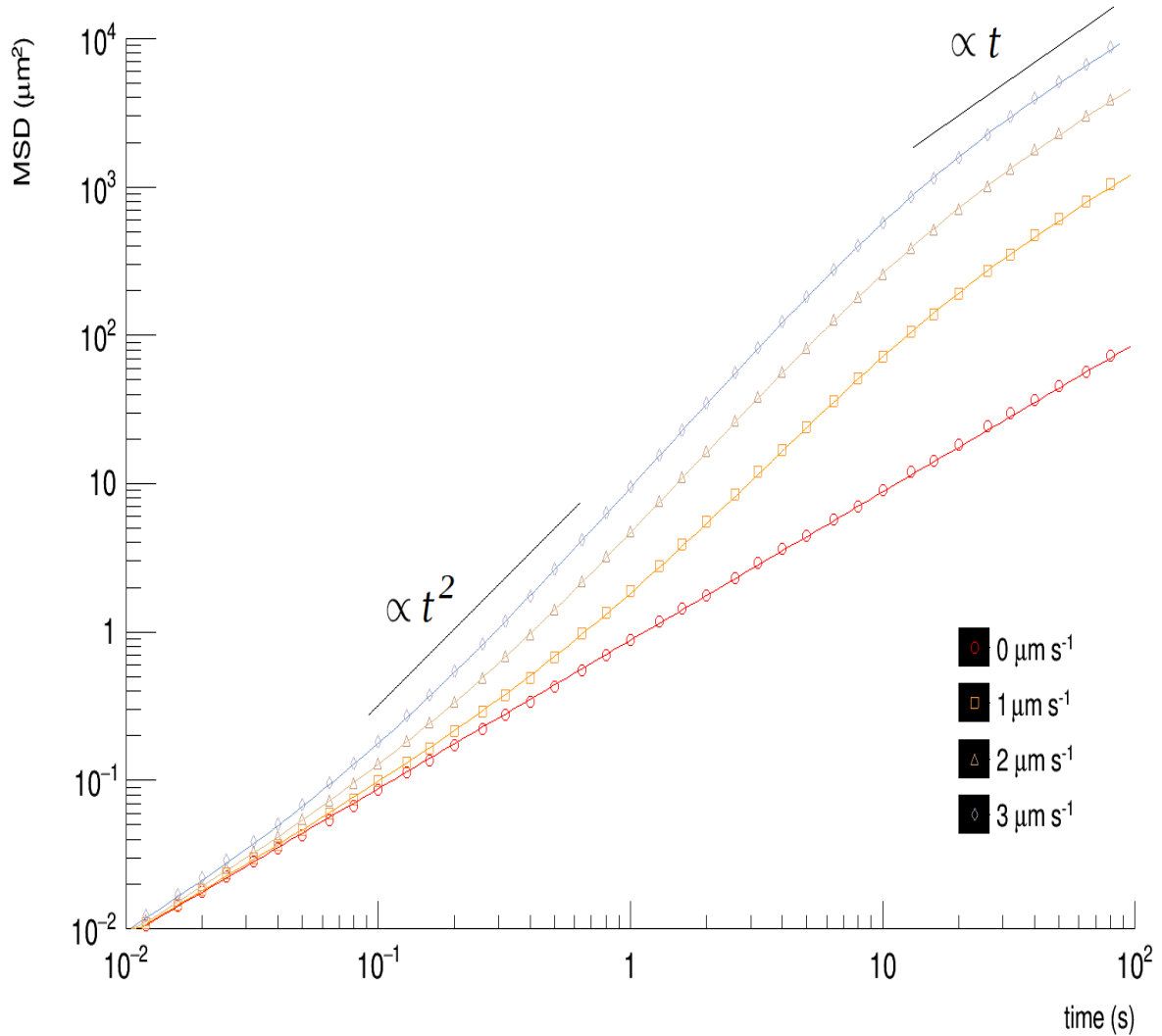The used parameters to run the simulation are $v = 1\frac{\mu m}{s}$, $\Delta t = 10^-4$ and $N = 10^3$.

Figure (4.2)   Mean square displacement in two dimensions of passive and active particles. The lines represent the theoretical values of the MSD while the markers the values of the simulation with drift velocity $v = 0$ μms^{-1} in red cyrcle, $v = 1$ μms^{-1} in yellow squares, $v = 2$ μms^{-1} in brown triangles , $v = 3$ $\mu m/s^{-1}$ in blue rhombus.
The motion of the active particle is ballistic on short time scales, $MSD \sim t^2$, for $t << \tau_r$, and becomes diffusive on a longer time scales, $MSD \sim t$, for $t >> \tau_r$.
The used parameters to run the simulation are $\Delta t = 10^-4$ and $N = 10^3$.

Chapter 5

Interaction with a wall

So far we have considered particles free to move everywhere. We are going to add two conditions. The first one is that the particles are confinded in a rectangular box of lenght L_x and L_y and their x and y position can vary between 0 and L_x and the L_y respectively. Along the x-axis we have the periodic boundary that if a particle exceeds the lenght of the box L_x or goes to a negative position it appears on the opposite side of the box. The second one is the presence of a boundary. Along the y-axis there is a planar vertical wall on both side. If a particle hits the wall it is reflected as showed in 5.1 .
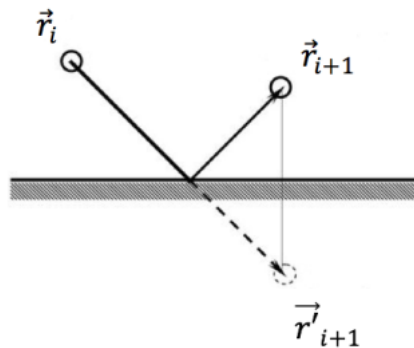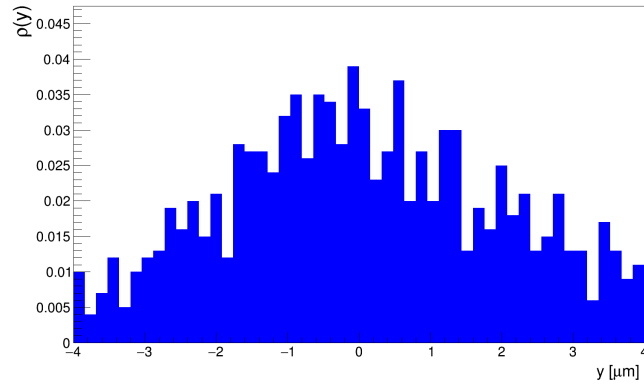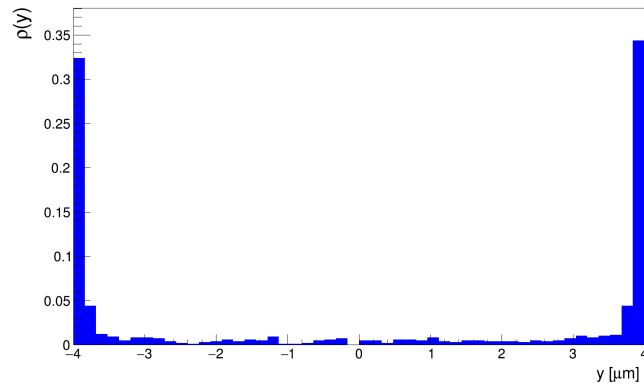

Figure (5.1)   [3]

The probability distribution of the y position $\rho(y)$ of the passive particles tends to a normal distribution.
For active particle $\rho(y)$ increases very stiply near the wall and decreases abrupt in the regions far away the wall, almost vanishing.
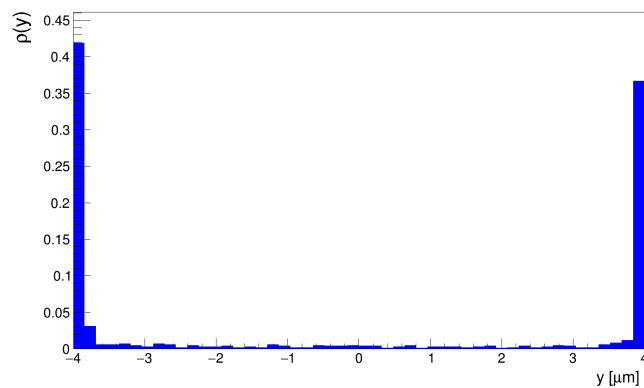The results are showed in Figure(5.2) and confirm our deductions.

(a)

(b)

(c)

Figure (5.2)   (a) $\rho(y)$ of passive particles, it tends to the Gaussian distribution.
(b) - (c) $\rho(y)$ of active particles, (b) $v = 5\mu m/s$ (c) $v = 10; \mu m/s$. We see how the probability that an active particle hits the bounday rises as v becomes bigger.
The total simulation time is 10 seconds with the presence of $N = 10^3$ particles.

Chapter 6

Interaction between particles

In this chaper we are going to work in two dimensions and suppose the existence of a pairwise potential $V(r)$ between the particles of the form :

$$V(r) = C \frac{\exp\left(-\frac{r}{r_0}\right)}{|r - r_0|}$$

where r is the distance between any two particles and C is a costant that gives the appropriate units dimensions to the potential and may set its order of magnitude. $V(r)$ takes higher values when the particles get closer and tends to infinity when the distance between them approaches r_0. This reflects the fact the particles cannot overlap.

In this chapter we consider the distance r between any two particle as the distance between the center of two circoference of ray r_0, which is the ray of the particles. [2]

The spatial coordinates refer thus to the one of the center of the circonference that the particle represents. Indeed for any two particles of coordinates (x_i, y_i) and (x_j, y_j) we have:

$$r = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} = \sqrt{(\Delta x)^2 + (\Delta y)^2}$$

We now define a new potential $U(r)$ introducing a cut-off distance r_{cut} , which allow us to reduce the number of iterations to compute among the particles:

$$\begin{cases} U(r) = V(r) - V(r_{cut}) & \text{for } r < r_{cut} \\ U(r) = 0 & \text{for } r \geq r_{cut} \end{cases}$$

thus:

$$U(r_{cut}) = 0$$

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[2]For the simulation of this chapter we used particles of a ray r_0 different from R.

$$F(r_{cut}) = 0$$

In this way there is no more the discontinuity jump at $r = r_{cut}$.
The total force acting on a particle is

$$\vec{F_i} = -\nabla_{\vec{r_i}} \sum_i^N U(r_{ij})$$

The force acting between each pair of two particles in two dimensions reduces to :

$$\vec{F_i} = -\nabla_{\vec{r_i}} U(r_{ij}) = -\left[\hat{i}\frac{\partial}{\partial x_i} + \hat{j}\frac{\partial}{\partial y_i}\right]U(r_{ij}) =$$

$$= -\frac{\partial U(r_{ij})}{\partial r_{ij}}\left[\hat{i}\frac{\partial r_{ij}}{\partial x_i} + \hat{j}\frac{\partial r_{ij}}{\partial y_i}\right] = -\frac{1}{r_{ij}}\frac{\partial U}{\partial r_{ij}}(\Delta x\hat{i} + \Delta y\hat{i})$$

where

$$\frac{\partial U(r_{ij})}{\partial r_{ij}} = -C\frac{e^{-\frac{r}{r_0}}}{|r - r_0|}\left(\frac{1}{r_0} + \frac{1}{r - r_0}\right)$$

$$\vec{F_x} = F_x\hat{i} = -\frac{1}{r_{ij}}\frac{\partial U}{\partial r_{ij}}\Delta x \; \hat{i}$$

$$\vec{F_y} = F_y\hat{j} = -\frac{1}{r_{ij}}\frac{\partial U}{\partial r_{ij}}\Delta y \; \hat{j}$$

We need to solve now then two equations of motion of active particles under the effect of a repulsive force $\vec{F} = (\; F_x \; \hat{i} \; , F_y \; \hat{i} \;)$:

$$\dot{x} = 2D_t\xi_x + \frac{F_x}{\gamma} + v\cos\varphi(t) \qquad\qquad (6.1)$$

$$\dot{y} = 2D_t\xi_y + \frac{F_y}{\gamma} + v\sin\varphi(t) \qquad\qquad (6.2)$$

The formal solution of equation (6.1) is:

$$x(t_0 + \Delta t) = x(t_0) + \int_{t_0}^{t_0+\Delta t} \left(\; 2D_t\xi_x(t) + v\cos\varphi + \frac{1}{\gamma}F_x \;\right)\mathrm{d}t$$

but since the force is time indipendet and we already know the solution in the absence of the potential, we can easily deduce the algorithm to simulate the particles position:

$$x(t_0 + \Delta t) = x(t_0) + \sqrt{2D_t\Delta t}\; \xi_x(t_0 + \Delta t) + \left(\; v\cos\varphi(t_0 + \Delta t) + \frac{1}{\gamma}F_x \;\right)\Delta t \qquad (6.3)$$
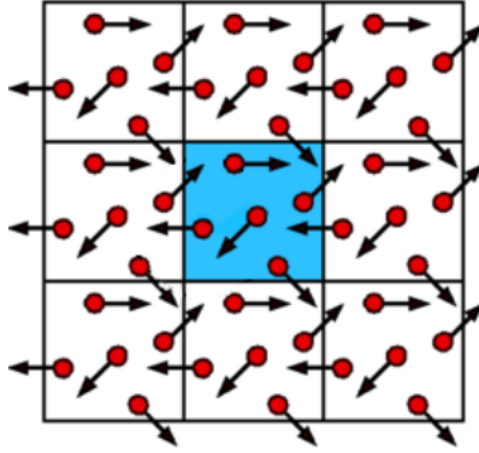
Figure (6.1)   Representation of the periodic conditon for the principle of minimum image convection.

In the same way:

$$y(t_0 + \Delta t) = y(t_0) + \sqrt{2D_t \Delta t} \ \xi_y(t_0 + \Delta t) + \left(v \cos \varphi(t_0 + \Delta t) + \frac{1}{\gamma} F_y \right) \Delta t \qquad (6.4)$$

To simulate the effect of the interactions between particles due the $U(r)$ pontetial, we started placing randomly 10^3 particles in a rectungal region of sides 50 μm and 80 μm. Actually we used an alogritmh to avoid to place two particles too close one to each other for in their initial position. We implemented the periodic boundary conditions for both sides of the box and a method called minimum image convection. We consider our box to be at the center of other 8 equal copies of our system, as summarized in figure (6.1). The principle of minimum image convection tell us to consider the interaction, of each particle in relation with the other, just with the clostest one of the 8 copies.

The ray r_0 of the particles is $r_0 = 0.1$ μm and their drift velocity is $v = 1\mu m s^{-1}$. We set a cutoff distance $r_{cut} = 5r_0$ and the value of C was chosen to be numerically equal to the numerical value of γ.

Figure (6.2) shows the results. The total simulation time is 10^2 seconds and we start to see the formation of cluster. We can try to visualize better this behaviour following the position of two particles belongig to the same cluseter. They should follow close path. Have a look on figure (6.3).

Note that we compute the value of the force between the particles at every fixed interval time Δt. We have a great limit on the simulation duration that we can reach. In fact we need a very little Δt in ordet to avoid that the particles get too close and thus get some huge unrealistc values of the force. Reducing the simulation step Δt forces us to make more iterations. Since all the simulations were performed using a personal computer,
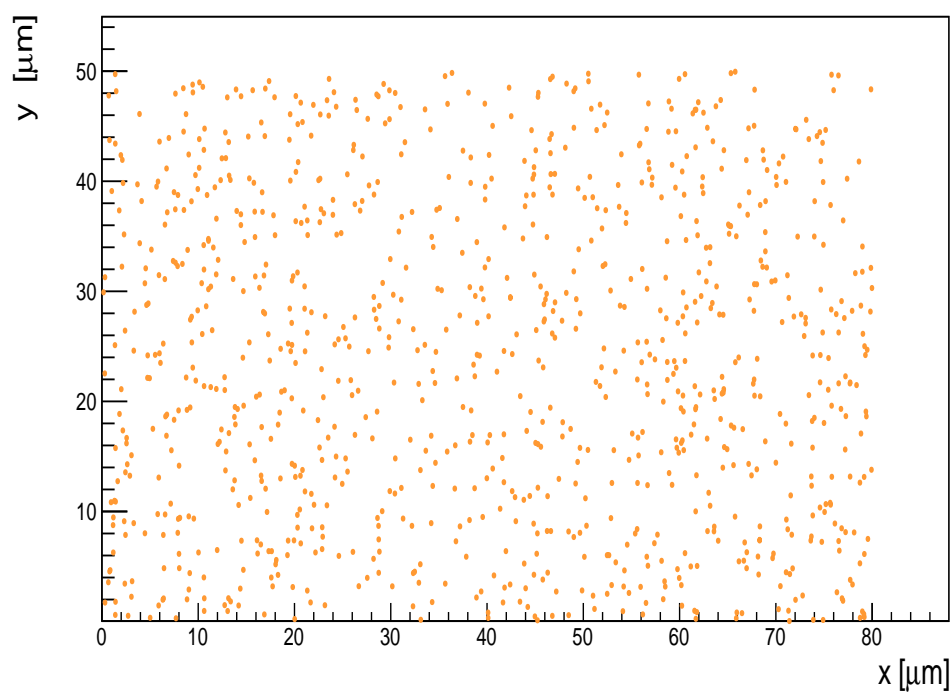
Figure (6.2)   Position of active particles under the effect of a repulsive potential after 10^2 seconds elapsed. The used values in the simulation are $N = 10^3$, $\Delta t = 10^{-3}$ and $v = 1\ \mu m s^{-1}$.
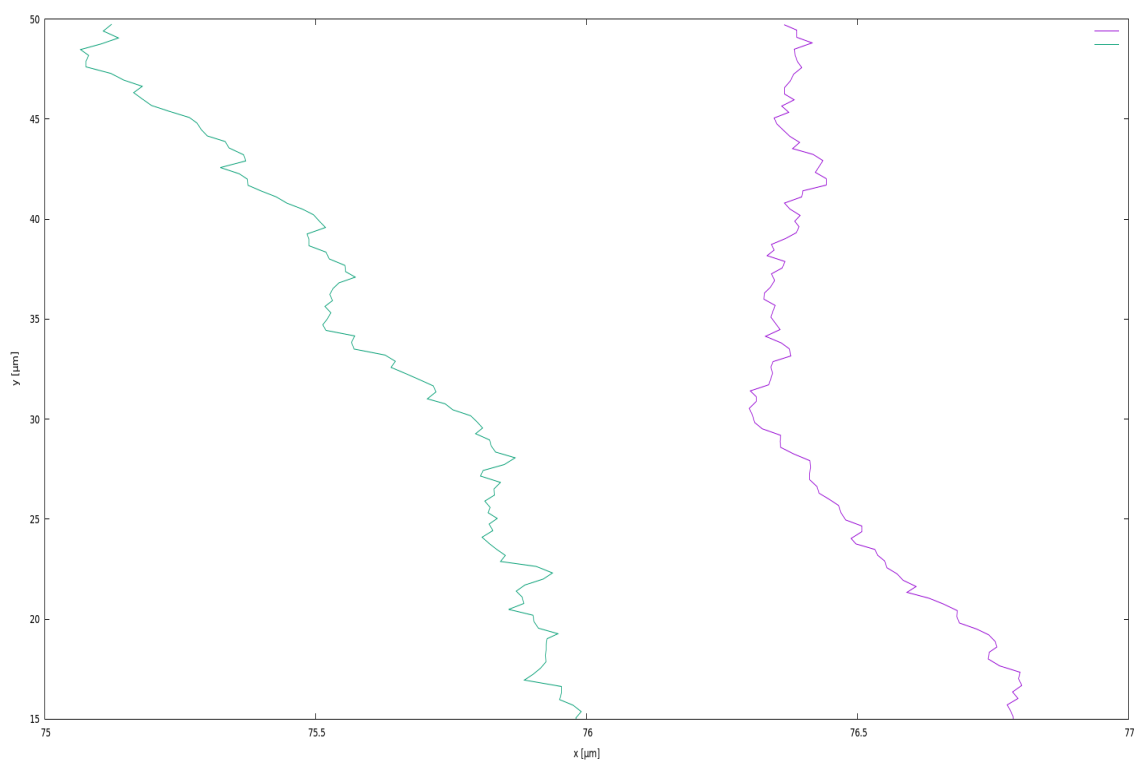
Figure (6.3)   Path followed by two different particles belongig to the same cluster.

our calculation power was really limited. In particulary our processor takes two hours to run the entire simulation of figure (6.2) and (6.3) and more ten times longer to reach 10^3 seconds of total simulation. It should be clear that the formation of real cluster would require more then few minutes, thus we cannot expect more then what we obtained from our work.

Chapter 7

Conclusions

We analyzed the differences in the collective dynamics of passive and active microparticles but we should also highlight the fact that nowdays scientists are able to directly observe and even manipulate objects of micrometer size. We can image an artificial robot, of micrometer size, whose task is to deliver some biological molecule to a region of the human body. Probably the biggest difficulty is that they have to deal with a huge number of particles and thus follow the single behaviour of each of them becomes very hard if not useless. Since the collective behaviour prevails, we focussed our study exactly on the collective properties of these microswimmers.

Furthermore we saw the stochastic nature of the equation which describes their dynamics and gave some models to simulate their behaviour.

We observed the mean square displacement in time and saw that it is purely diffusive in the case of passive particles and proportional to a constant term called diffusion coefficient. This term is proportional to the temperature of the fluid and inversely proportional to the Stoke's coefficient. It is quite easy to understand why. Higher temperature means higher molecular agitation of the fluid molecules. Thus the intensity and the number of the collisions, between the molecules of the fluid and the particles, increase. As an obvious effect the particles' displacement increases too. The Stoke's coefficient that we call γ depends on the shape of the object and it is proportional to the ray of the particle in the spherical case. For smaller ray γ decreases too and the friction force of the fluid becomes smaller. Thus we have again a bigger displacement of the particles. The considerations made on the coefficients are still valid in the case of active particles, but here the drift velocity plays a fundamental role. In fact for active particles the mean square displacement is ballistic for times smaller than the inverse of the rotational diffusion coefficient, τ_r, and diffusive for larger time. In this case we have an *effective* diffusion coefficient which is higher than in the passive case. This is quite obvious since the displacement of self-propelling particles is clearly higher than the passive ones.

The quadratic behaviour reflects the fact that as the simulations starts, and so the

particles start to move, they all swim away from the initial position where they were placed. This means that the mean square displacement grows fast, much faster that in case of passive particles. After τ_r seconds are elapsed the direction of the velocity starts to point toward some aleatory region. This means that now the particles can get closer to their initial position. Recalling the very definition of the mean square displacement, help us to understand this process. Looking at our simulations we see that the transition between the two regimes appears quite rapid. It is important to note that it happens always at the same small region near the value of τ_r. This is because for every simulation we used the same value of D_r, which determines the time scale when the particles lose the information about their initial position.

A distinguishing characteristic of active particles is the probability distribution density of the position under the presence of a planar repulsive boundary. It shows us their tendency to accumulate on it. This is because there is an asymmetry between the process of leaving and approaching the boundary. When a particle leaves the wall, it swims away from it, when it is approaches it, the particle gets stuck at boundary until the direction of the velocity orientates toward the interior. These processes produce a propensy of the particles to accumulate near the wall. Instead passive particles, in thermodynamic equilibrium with the environment, remain homogeneous distributed in space even in the presence of a wall.

Under the effect of a pairwise repulsive potential active particles form agglomerate. If we think just about two active particles, they clearly move away one from each other until they reach the cutoff distance of the potential and so the distance between them remains constant. When we consider a higher number of particles they show up a tendency to form clusters. In this situation two or more particles can spontaneously become closer as a result of the net force acting on them. Thus, there are some region where the density of particles is higher. This random gathering process goes on until they create a kind of small cluster. Now the cluster itself acts as repulsive boundary and in an analogous process to the one described in the presence of a repulsive wall, more and more particles accumulate on it. For the same reason we explained before, clustering cannot happen to passive particles.

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