Coagulation Process of Escaping Bubbles and Parallel Simulation

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I. Introduction.

Consider a liquid of volume V at a given temperature T and pressure p containing some gas of volume FV . As the temperature rises, minimization of the free energy favors the escape of dissolved gasses .Rather then evaporating only from the surface this can happens via bubble formation. Due to a surface energy barrier only bubbles of radius $a > a_{min}$ form. If we have just few large bubbles the latter grow further and the gas quickly escapes.

We consider however the case where there are many, small, bubbles with some size distribution f(a). We will not address the formation of these bubbles and their possible instabilities. We just assume that some mechanism produced the above bubble population and that these are stable over time scales relevant to our ensuing discussions. The distribution $f(a) = f(a;t = 0)$ is thus provides the initial condition for the time evolution of the bubble population on which we focus.

Stokes' viscous drag $6\pi\eta au$ and the $g\rho 4\pi/3a^3$ buoyancy with ρ the density of the liquid fix the upward drift speed of a bubble of radius a (with the gas density neglected) :

$$u = \frac{2g\rho a^2}{9\eta} = k_u a^2. \tag{1}$$

The viscosity of most liquids at room temperature is: $\eta \sim 10^{-3}-1$ Poise and the density is O(1) . A single small bubble of radius of 10 microns $\sim 10^{-3}$ cm requires 1/2 an hours to drift to the top of a 20 cm tall cylinder full of water when no convective/ turbulent effects are present and Stokes law for laminar flow holds. (The 1% pressure variation and slight deformations of the moving bubbles have small effects)

In the realistic case when many bubbles are present the bubble escape rates are modified by at least two mechanisms: The first , "local" effect is the coalescence of colliding bubbles. Larger bubbles are, according to Eq 1, faster than smaller bubbles and will overtake those as the latter drift slowly upwards. The resulting larger bubble formed has a larger cross-section for colliding with and further picking other bubbles which it is even more likely to overtake now being faster as well. The net effect is to accelerate the escape of all the gas in the bubbles. Our focus here is precisely this "Avalanche like" effect of bubble. There is a second "long range " effect. It is the draging along of slower bubbles by the common "collective" flow in the vertical direction generated by the rest of the bubbles and in addition weaker transverse forces attracting the bubbles towards each other.

We start by estimating the second effect . While it could be of a genuine many body nature, we treat it first as due to pairwise bubble bubble interactions. Since we find that for a generic bubble these sum up to a force much smaller than the "one body" Stokes drag force this approximation is justified .

Let $F_{1.2}(a_1, a_2; u_1 - u_2)$ be the force exerted on bubble #1 with velocity u_1 and radius a_1 by bubble #2 with radius a_2 at a distance $R = |r_1 - r_2|$ away and moving with velocity u_2. By reciprocity (Newton's third law) it is symmetric in 1 and 2. Just as in the derivation of Stokes law (Joos), $F_{1,2}$ obtains by integrating over the surface of bubble #1 the shear stresses exerted, due to the finite viscosity, by the velocity field generated by bubble #2 moving vertically elative to bubble #2 with velocity $(u_2 - u_1)$. The velocity field falls like $1/R$ the and the viscose force is due to gradients of the latter. Hence from dimensional and symmetry arguments we expect that :

$$F_{1,2} = \frac{c\eta a_1^2 a_2^2 (u_1 - u_2)}{R^3}. \tag{2}$$

with c a numerical coefficient, analog to the 6π in Stokes law $F_{11} = 6\pi\eta a u_1$ for the "self" force of a single bubble. For a crude estimate assume that all bubbles to have the same radius a yet allow different velocities. We then find that

$$F_{1,2} \approx c\eta u a \Big[\frac{a}{|r_1 - r_2|}\Big]^3.$$

Integrating over all other bubbles within say a sphere of radius R surrounding bubble #1 we find that:

$$\frac{F_{collective}}{F_{Stokes}} = \sum_i \frac{F_{1,i}}{F_{stokes}} < F\ln(\frac{R}{a}) \ll 1 \tag{3}$$

With the volume fraction of the bubbles $F \ll 1$ this is then a small correction to Stokes force of an individual bubble.

Since bubble faster than the bubble #1 accelerate its motion and slower bubble decelerate itself there are many cancellation in the last sum. Indeed Newton's third law prevents the complete set of bubbles from self- accelerating upward, just as the Baron Minchhausen could not lift himself by his boot-straps. Still $F(collective)$ tends to equalize the speeds all bubbles- exactly the opposite of $F(stokes)$ which as indicated above generates very disparate velocities for bubbles with different radiuses.

These velocity differences are at the crux of the bubble coalescence which is out main focus.by allowing faster, bigger bubbles to overtake slower smaller ones . Thus it was important to verify that the smaller collective force will not undermine it by equalizing all speeds.

There can be yet another more subtle interplay between the long range two body forces and the local bubble-bubble coalescence avalanche of interest. The transverse (x, y) component of the forces are attractive and tend to bring bubbles closer to each other in the x, y plane. Thus a spatial bubble distribution which is uniform in x, y can transform to a configuration where translational invariance in the (x, y) plane is spontaneously broken. In the new "phase" we have enhanced bubble densities along vertical filaments at specific (x_i, y_i) locations. The increased local density will shorten the mean free path for collisions of bubbles moving in the vertical,z, direction in each filament, further accelerating the bubble avalanche and escape. We will reconsider this issue in our last section.

II. Bubble coalescence avalanche , some general considerations..

Colliding bubbles often coalesce into bigger bubbles with faster upward motion. These pick up more bubbles , get bigger yet , move faster, etc etc .The resulting "upward avalanche" allows (most of) the gas to escape in a time of order of the average time for bubble-bubble collision .

So long as the mean free path for bubble collisions l is much smaller than the height H of the container the evolution of the above avalanche is drastically simplified. While a generic bubble suffered k collisions and its speed has increases by $\sim k^{2/3}$ it moves only a small fraction kl/H of the total height. During this time the distribution $f(a)$ may significantly shift towards larger a values. Yet, apart from small edge regions: $z < kl$ and $H - kl < z < H$, the bubble distribution does not vary with the height z.

Using an average b-b cross section $\sigma \approx 4\pi a^2$ in the definition of the mean free path l for b-b collision: $l = (n\sigma)^{-1}$ with $n = F/4\pi/3a^3$the average bubble number density yields :

$$l = \frac{a}{3F} \tag{4}$$

we mainly focus on the period when

$$l \ll H \quad \text{or} \quad a \ll 3FH$$

with H the container's height. By the time that the evolved distribution $f(a;t)$ starts saturating this bound we have large bubbles of average radius

$$\langle a(t)\rangle = \frac{\int f(a;t)a\ da}{\int f(a;t)da} \sim 3FH \tag{5}$$

Thus $\langle a\rangle \sim 0.3$ cm for $H \sim 20cm$ and $F \sim 1/2\%$, and such bubbles will quickly escape independent on any further growth.

We discuss next the time evolution of the distribution of bubble sizes $f(a;t)$ during the stage when eq Cond above is satisfied so that we can neglect any variations with height (z). The evolution is driven by larger bubbles of radius a' overtaking smaller bubbles of radius a" and smaller velocities $u'' \sim a''^2 < u' \sim a'^2$. The collision could preserve the bubbles which would emerge from it with changed vector velocities . However the buoyancy and viscous drag quickly restore the final bubble velocities to upward drifts with the same speeds u' and u'' fixed via Eq 1 by a' and a''. The relevant relaxation time is given by the ratio of the coefficient of the inertial term , $m =$ effective bubble mass $= 4\pi/3a^3\rho$, and the coefficient of the viscous term that is $6\pi\eta a$:

$$\tau \sim \frac{2}{9}\rho\frac{a^2}{\eta} \tag{6}$$

The key point is that tau is shorter than the average time it takes a bubble to suffer another collision, $t_{collision}$. The latter is given by the mean free path for bubble collision divided by the relative speed:

$$t_{collison} \sim l/u \sim \frac{a/F}{2a^2 g\rho/(9\eta)} \tag{7}$$

Indeed the ratio

$$t_{collision}/\tau = \frac{4}{81}a^3\rho^2\eta^2 gF^{-1} \tag{8}$$

is rather large $\sim 10^2$ for $a \sim 10^{-3}$ cm, $F \sim 1\%$ and viscosities η as small as 10^{-3} in cgs units. Hence most of the time the bubbles travel essentially upward with the "asymptotic" velocity of $u = 2/9g\rho a^2/\eta$. Also for these low speeds bubble - bubble collisions are unlikely to result in bubble fragmentation is unlikely.

The only relevant collisions then involve merges of the two colliding bubbles into a single bubble of radius a and volume $v = v' + v''$- the sum of the volumes of its "parents" so that:

$$a = (a'^3 + a''^3)^{1/3}. \tag{9}$$

The probability p that a merge will occur in a collision of two bubbles will in general depend, even after averaging over impact parameters, on a', a'' and the corresponding speeds u' and u". As a first approximation we take p to be a constant.

Due to the energy barrier imposed by topology change two bubbles stuck together may require some extra time t_{merge} to actually physically merge into a single bubble

. We focus in this section on the limit "instantaneous" case when t_{merge} is (much) shorter than $Rt_{collision}$- the time required for an average bubble to collide . In Sec III we will consider the other limit $Rt_{merge} \gg Rt_{collision}$ namely bubbles that maintain their identity but stick together into clusters or "Super=bubble"- again accelerating gas escape.

We now estimate $t_{collison}$. The time required for a bigger-bubble with drift speed u' to overtake a smaller, slower bubble with speed u'' at a distance l above it is $t \sim l/(u' - u'')$. The average $Rt_{collision}$ is then roughly

$$t_{collision} \sim l/\Delta(u) \tag{10}$$

where $\Delta(u)$ is the width of the u distribution fixed (via Eq 1) by the width of the distribution of radii a. If the latter are not strongly peaked around one particular a_0 (or corresponding u_0) we can approximate $\Delta(u) \sim \langle u \rangle$. Using the above l and u we find that the average time required for the first collision is:

$$t_{collision} = \eta/F\langle a \rangle. \tag{11}$$

and for $F \sim 10^{-2}$ and $\langle a \rangle = 10^{-3}$ cm we find $t_{collision} \sim 100$ sec .

Since merges conserve volume we can use instead of a, the bubble volume v and denote by $f(v;t)$ the fraction of bubbles of volumes in the interval $v - -v + dv$. Throughout the evolution of interest no appreciable amount of bubbles escapes. The total volume is conserved and :

$$\int f(v;t)v \; dv = FV \tag{12}$$

remains constant.

The above $f(v)$ is similar to the " distribution functions for nuclear particles, $f(x)$, the # density of "partons" carrying a fraction x of the total hadron's momentum used for collisions at high energy and large momentum transfer(Q) collisions. The evolution of $f(x;Q)$ in a "time" $\tau \sim \ln(Q^2)$, tends to split partons pushing the distribution towards $x = 0$ - the opposite of merges and generation of bigger bubbles here..

III. Social-economic mergers - possible analogs of merging bubbles?

An interesting possible analog is the social-economic phenomena of merging of corporations tribes nations etc. into larger units. These are generally controlled by very many factors-efficiency, competition, and even human emotions making them, as all social phenomena, far more complicated than the (relatively!) simple bubble merges. There are ,however, common features suggesting some analogy between the two types of merges . We present below a model of merging one dimensional bubbles which in a well defined sense belongs in the same "universality class" as a particular class of social-economic merges.

To proceed let us consider then the following (truly simplified) model of competing merging commercial units -aka "companies". Let us assume that all the companies in question specialize in producing and selling the same product so that analogy with the homologus bubbles is concieveable possible. This also allows ranking all these companieson a one dimensional 'success" axis denoted by u the analogy of the upward speed of bubbles u_i .

This success/velocity depends on (at least..) two counteracting elements:

a) the total resources financial, technological, human etc. of each company. These resources provide the upward driving force which generate the bubbles velocity (or "success" of companies). It is suggestive to map the "resources" onto the volumes of the bubbles- which indeed determine the Buoyancy -upward driving force. Further, upon merging the two companies the resources - just like volumes- add up.

b) Many effects oppose quick development and tend to reduce "success". These include external red tape , internal bureaucracy, required R@D expenses etc. Note that most of these increase at a slower rate then the total resources. Thus upon merging of two companies which are doing the same thing -the external red tape @ R&D and even the internal bureaucracy can remain almost the same. All these effects are modelled here by the frictional viscous forces opposing and slowing down the upward motion of the bubbles. These indeed grow more slowly then the volume or corresponding buoyant force propelling the bubbles upward. Thus in the example above, merging two equal bubbles v'=v"=v doubles the volume but the viscose drag -proportional to the bubble's radius $a \sim v^{1/3}$ increases only by $2^{1/3}$! The particular numbers reflect the specific physical model of slowly drifting bubbles in three dimensions generating a laminar flow. Drifting bubbles in other dimensions and modified viscous forces may better model the social-economic merges.

The feature that when a slower bubble is overtaken by a larger faster one they tend merge is common to all bubble models considered here. It is the analog of what generally happens in the social-economic case. Thus assume that company A' attained a larger success (i.e. "velocity") u then company A" in doing the same thing. (say-developing/producing/selling the same product). Company A" can then no longer compete with A' and it makes economic sense for both companies to merge. The impetus to do so and the rate at which it is likely to happen, is faster the bigger is the difference between the corresponding "successes u' and u''s. This is modeled in the drifting bubble case by having the time required for bubble -bubble collision:

$$t_{collison} \sim \frac{1}{u' - u''}. \tag{13}$$

In all bubbles models the upward speed is proportional to some (positive) power of the volume: $u \sim v^b$. This introduces into the rate for bubble collisions and merges the factor $t^{-1}_{collison} \sim u' - u'' \sim v'^b - v''^b$.

Locality namely having only nearby bubble in physical contact merge applies to bubbles. It introduced above the geometric "cross section area for $b'-b''$ collision"

$$\sigma(b'-b'')=\pi(a'+a'')^2\sim(v'^{1/3}+v''^{1/3})^2 \qquad (14)$$

as an extra factor in the rate of merges of bubbles with volumes $v'v''$:

$$\Gamma_{merge}(b'-b'')\sim(u'-u'')\sigma(b'-b''). \qquad (15)$$

In D rather than three dimensional space, eq 15 is replaced by

$$\sigma(b'-b'')\sim(v'^{1/D}+v''^{1/D})^{(D-1)}. \qquad (16)$$

There is no clear counterpart of this locality in merges in a more "Global" economy. However in the limit of short relaxation time we saw that the bubble motion is effectively one dimensional -upward along the z axis . Further for short collision length (relative to system size) also the separation along the z axis $|z'-z''|$ no longer appears in the bubble evolution derived next and locality no longer prevents a useful analogy between physical bubble and social-economic mergers . We thus continue discussing in parallel the two types of merges specializing later to individual cases.

IV. The time evolution equation:

We next derive the Boltzmann like "Master" equation– the Smoluchowski coagulation equation when applied to merging bubbles. Consider the short time interval dt between t and $t+dt$ .During this time bubbles of volume v' can merge with nearby- at a distance $dz=(u'-u'')dt$ above- smaller and slower bubbles of volume v'' forming a new bubble of volume $v=v'+v''$. The rate for that is given by the product of the number densities $n(v')$ and $n(v'')$ of bubbles with volumes v' and v'' respectively and the cross section $p\pi(a'+a'')^2$ for merging of such bubbles. During dt the effective target presented to the v' bubbles by the smaller v'' bubbles is "thin" (of thickness $dz=(u'-u'')dt$) and "shadowing" i.e. multiple merge, effects are negligible .

These considerations than lead to the time evolution of f(v;t) :

$$\frac{df(v;t)}{dt}=cp\int dv'\int dv''f(v';t)f(v'';t)(v'^{1/3}+v''^{1/3})^2$$
$$(v'^{2/3}-v''^{2/3})[\delta(v-v'-v'')-\delta(v-v')-\delta(v-v'')] \qquad (17)$$

Since $v'>v''$, the v''integration is nested in the v' integration and $a=(3v/4\pi)^{1/3}$ was used to express the relative velocity$u(v')-u(v'')$ in Eq 1 and collision cross-section Eq3 in terms of the volumes v' and v''. This fixes the (dimensionful!) constant c in Eq. 5 to be $c\sim 0.60g\rho/\eta$.

Integrating over v the sum of the three delta functions makes the r.h.s vanish and we obtain:

$$d/dt\int dv.vf(v,t)=0 \qquad (18)$$

Thus the evolution indeed preserves the total volume of bubbles given by Eq 13 above .

Integrating out the three δ functions and seperating the terms obtained we find:

$$\frac{df(v,t)}{dt}=cp[\int dv'\Theta(v-v')\Theta(2v'-v)$$
$$\times f(v';t)f(v-v';t)(v'^{1/3}+(v-v')^{1/3})^2$$
$$\times(v'^{2/3}-(v-v')^{2/3})$$
$$-f(v,t)[\int dv'f(v';t)\Theta(v-v')(v^{1/3}+v'^{1/3})^2$$
$$\times(v^{2/3}-v'^{2/3})] \qquad (19)$$

The two θ functions in the first term of Eq.6 reflect the $v>v'>v''$ ordering in the first term in Eq 5 (corresponding to $\delta(v-v'-v'')$. The two terms generated by the second and third δ functions in Eq 5 were collapsed into the single last term in Eq 6 by combining the $v'>v$ and $v'<v$ integrals into one unrestricted v' integral. We added the absolute value to $v^{2/3}-v'^{2/3}\sim(u-u')$ ensuring a positive relative velocity so that the larger bubble indeed moves faster and does overtake the slower, smaller bubble.

The evolution above is a special case of the Smoluchowski coagulation equation of the following general form:

$$df(v,t)/dt=\int dv'\int dv''K(v;v'v'')f(v',t)f(v'',t) \qquad (20)$$

With K a symmetric (in $v', v"$) kernel. In the present case it includes the three delta functions, the merge cross section ($\sim c(v'^{1/3}+v"^{1/3})^2$, and the relative velocity $\sim(v'^{2/3}-v"^{2/3})$.

Given any initial volume distribution $f(v;t=0)$ this nonlinear integral-differential Eq.6 fixes $f(v,t)$ at all times $t>0$, the function $f(v;t=0)$ is determined by the physics of initial bubble formation. This physics- not addressed here- does fix the minimal (critical), bubble size v_0 and the spread of volumes critical to subsequent mergers. At a time $t\gg t_{collison}$ later repeated bubble merges have occurred.

It may useful sometimes to consider instead of $f(v,t)$ above, the fraction of the total bubble volume in bubbles of sizes between $v$and $v+dv$, dimensionless $g(v;t)=vf(v;t)$. It keeps shifting towards higher v values as bigger bubbles keep forming at the expense of the smaller bubbles which keep disappearing in merges.

It is instructive to see this in a simpler case of "one dimensional" bubbles. While difficult to realize physically it may be applicable to certain cases of economic merges. Here the bubbles are not only restricted to move (up) along the z axis but are truly one dimensional. Thus the length a of each bubble replaces the volume $v\sim a^D$ is linear in a for $D=1$. The probability for mergeres is taken to be unity whenever one needle shaped bubble overtakes the other .Also since the cross sectional area is fixed we assume that the viscose force, linear in v, is independent of a. Taking again the buoyant force to be $\sim v=a$ we find that the upward drift velocity is also

$u = cv$. The evolution equation then becomes:

$$\frac{df(v,t)}{dt} = c[\int {v_0}^{v/2} dv' f(v') f(v-v')(v-2v') - \int {v_0}^{\infty} f(v) f(v')|v-v'|] \quad (21)$$

The second term accounts for disappearance of bubbles in a given v-v+dv interval by overtaking a slower bubble with a lower volume or by being overtaken by a faster bubble.

While this seems far simpler than the original equation 20 it is actually rather similar. Thus a lower bound to the rate of bubble growth as dictated by Eq. 20, obtains by replacing the factor $(v'^{1/3}+v''^{1/3})^2$ by the smaller $v'^{2/3}+v''^{2/3}$. The complete kernel then becomes $\sim v'^{4/3} - v''^{4/3}$ and we find an equation rather similar to Eq.19. The only difference being that the factor $(v-2v')$ in the first term and $|v-v'|$ in the second are replaced by the more general $(v-v')^b - v'^b$ or $|v^b - v'^b|$ with $b = 4/3$ rather than 1.

V. Analytic and Numerical Solutions of the Bubble Merge Equations

We cannot have an asymptotic ($t \gg t_{collison}$) stationary final distribution as merges cause an exponential growth of bubble sizes and corresponding decrease of bubble numbers preserving the total bubbles volume . Optimally we may have universal asymptotic time dependence affected only by a few features of the initial $f(v.t=0)$. Thus we can try an ansatz with the above growth /decrease pattern built in:

$$f(v;t) \sim \exp[-at/t_{merge} a(v/v_0)] / \exp[a(t/t_{merge})]. (22)$$

where the only information from the initial state is v_0 , the threshold volume for bubbles formation

MUCH MORE IS NEEDED HERE. /***/
This part is done by Yuhe Wang

There are two approaches to solve this problem numerically: one is to solve this differential and integral equation directly, which is hard and messy, but may takes little time to run. The other approach is to apply molecular dynamics to simulate every bubble,and then extract the statistics data. It's more accurate and easier to write code, but may cost a long CPU time due to the large number of particles. Considering the complexity of eq-(17), it will be a good idea to obtain numerical data from approach two and test the theory we developed.

Imagine that there is a container with bottom size $L \times L$ and height H. At initial time, the bottom part of the container is uniformly filled with bubbles of different radius a, which obeys a certain probability distribution $\tilde{f}(a)$ such as Uniform, Gaussian, Poisson, etc. As discussed in section II, Each bubble will gain a velocity u determined by eq-(1) within a time τ_0 negligible compared to the time step Δt. Due to the difference of velocities, the faster bubbles will catch up with the slower ones and collide with them. To simplify our simulation, we assume that the bubbles are so sticky that they fuse into one big bubble immediately after collision, and accelerates to a new velocity quickly.

Then the model of the program is rather simple: (1)move up every bubble at their velocity u_i, i.e. $z_i += u_i \Delta t$, (2)detect overlap of particles, (3)If any n bubbles overlap with each other, they forms a new bubble with $a = (\sum_{i=1}^{n} {a_i}^3)^{1/3}$, and new velocity $u = k_u a^2$,(4)output the position and radius of all bubbles for analysis, (5)repeat from (1) until the bubble number distribution $f(a,t)$ approaches an asymptotic form.

Here are the initial settings of our simulation: The bubble number $N_{max} = 40,000$; $\tilde{f}(a)$ is Gaussian or Uniform distribution so $f(a,t_0) = N_{max}\tilde{f}(a)$; $\bar{a}(t = t_0) = 0.4mm$, $\sigma_0(t=t_0) = 0.1mm$; $L = 80mm, H = 4000mm$,broad and high enough that no bubble will escape from the container, making the total volume conserved.

The velocity coefficient k_u and time step Δt needs dedicated choosing. The average distance bubbles move during one time step Δt must be much less than $\bar{a}$, say

$$u(\bar{a})dt = k_u \bar{a}^2 \Delta t \leq 0.05\bar{a}$$

to guarantee accuracy. Then we got $k_u \Delta t \leq 0.05/\bar{a} = 0.125mm^{-1}$. To be safe, we choose $k_u \Delta t = 0.08mm^{-1}$. Actually, we don't have to specify k_u and Δt respectively because we only need their product in the simulation.

It's a challenging task to simulate N_{max}=40,000 bubbles at the same time because the traditional CPU based simulation executes codes in series, which may cost an unbearable long running time. To improve efficiency, we turned to employ Nvidia's latest GPU parallel computation technology CUDA instead. The most time-costing part is the overlap detection because theoretically you have to test $N(N-1)/2 = 8 \times 10^8$ times for each step. One accelerating trick is to sort all bubbles by their height(using CUDA Thrust lib), and then for bubble i, we only detect bubbles whose height within $[z_i - 2a_i, z_i + 2a_i]$ since farther bubbles can never overlap. Meanwhile, this trick reduces the correlation between bubbles, making it possible to develop a fast parallel algorithm. By employing GPU parallel computation and above optimization, we can reduce the running time of a 40,000 bubbles and 10,000 step simulation to 3.5 minutes on a laptop(CPU i7 3630QM, GPU GT650M). Besides using Origin and Matlab script, We also developed a software to visualize and analyse the simulation data. All the programs can be accessed at http://physics.wustl.edu/zohar/group/projects/bubble/index.html (URL1)

The initial distribution will significantly affects the time evolution, but there're also common features irrelevant to initial settings.

i) Gaussian initial distribution:

figure 1(a) shows the time evolution of total bubble numbers N, which seems decreasing exponentially. Applying the fitting formula in Origin

$$y = y_0 + Ae^{-t/\tau}, \tag{23}$$

we got $y_0 = 6374, A = 33468, \tau = 8.8$, and the corresponding function is well fitted with the data points.

Figure 1(b) shows the time evolution of the mean radius $\bar{a} = (\sum_{i=1}^{N} a_i)/N$, which also obey the exponential formula (), but yields a negative A. The corresponding parameters are $y_0 = 0.581, A = -0.185, \tau = 15.85$.

Figure 1(c) shows the time evolution of the deviation of the radius, which is defined as

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N} (a_i - \bar{a})^2}{N}}$$

It has a similar behavior as $\bar{a}$. Its parameters are $y_0 = 0.352, A = -0.272, \tau = 16.01$.

The distribution function $f(a,t)$ is shown as figure 1(d). It starts from a sharp symmetric Gaussian form to a flat asymmetric distribution. It decreases very fast at the beginning due to the dramatic collision, and then slows down because the bubbles becomes sparser and sparser due to the difference of velocities. The distribution becomes wider and asymmetric as the portion of large bubbles increase, hence the average and the deviation both become larger, coinciding with figure 1(b) and 1(c). The color contour graph of $p = f(a,t)/N(t)$(figure 1(e)) shows the most probable radius vividly: the brightest $a_b(t)$ only increases a little and then remains constant. It's reasonable because some small bubbles are initialized under large bubbles and never have the chance to catch up with others. Obviously, the most probable radius $a_b(t)$ falls far behind the average radius $\bar{a}(t)$.

ii) Uniform initial distribution:

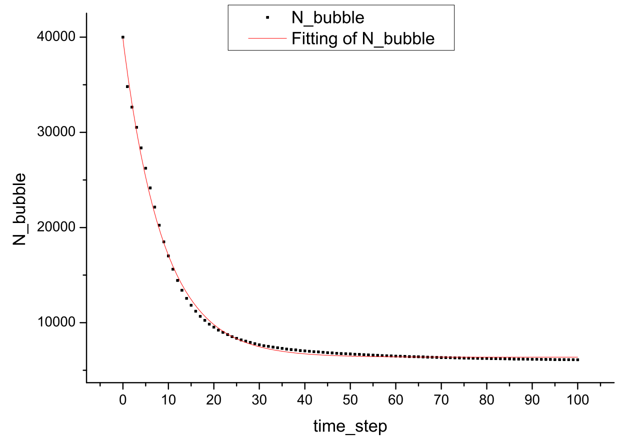
figure 2(a) shows the time evolution of bubble numbers N, which also seems decreasing exponentially. Applying the fitting formula () we got $y_0 = 6433, A = 34350, \tau = 12.85$, and a nice curve well fitted with the data points.

Figure 2(b) shows the time evolution of the mean radius $\bar{a}$, which also obeys the exponential formula (). The corresponding fitting parameters are $y_0 = 0.589, A = -0.199, \tau = 23.45$

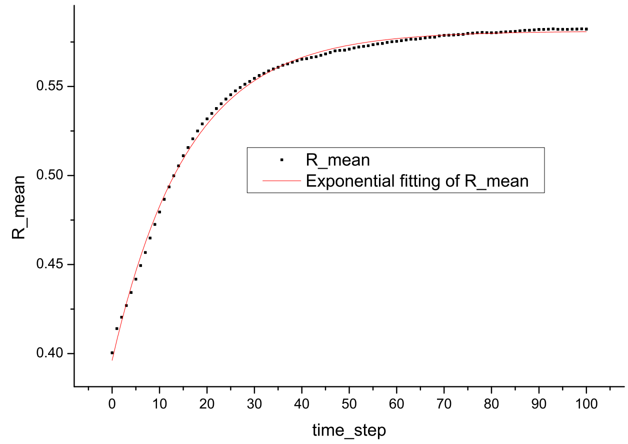
Figure 2(c) shows the time evolution of the deviation of the radius σ, which has a similar behavior as $\bar{a}$. Its fitting parameters are $y_0 = 0.315, A = -0.279, \tau = 21.64$.

The distribution function $f(a,t)$is shown as figure 2(d). It's similar to figure 1(d) corresponding to Gaussian initial form. The main part decreases exponentially, and evolves from a sharp symmetric distribution to flat asymmetric one, with large a extended. Figure 2(e) reveals that even the most probable radius has the same behaviour.

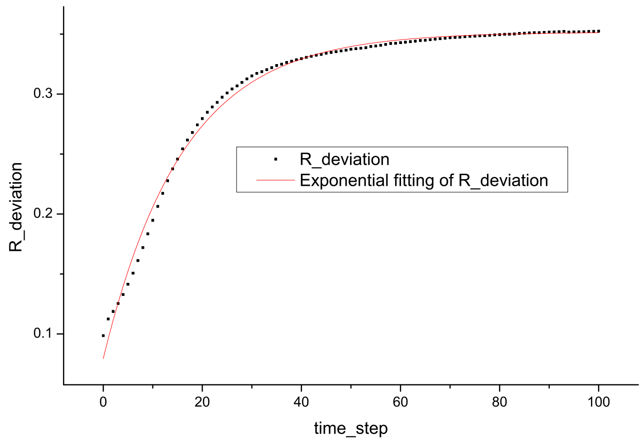
iii) more different initial distributions Figure 3 and **??** shows two evolutions of quite different initial distributions, two Gaussians and two Deltas respectively. It turns



(a)exponential fitting of $N(t)$



(b)exponential fitting of $\bar{a}(t)$

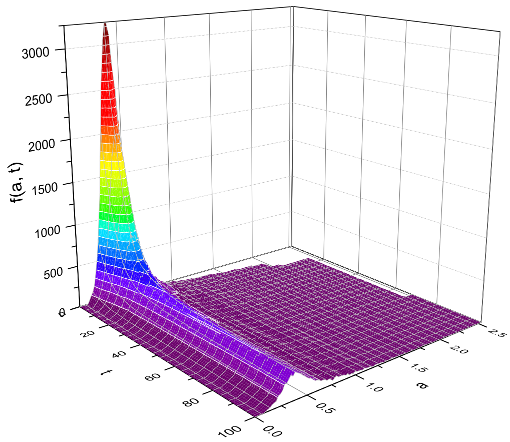


(c)exponential fitting of $\sigma(t)$

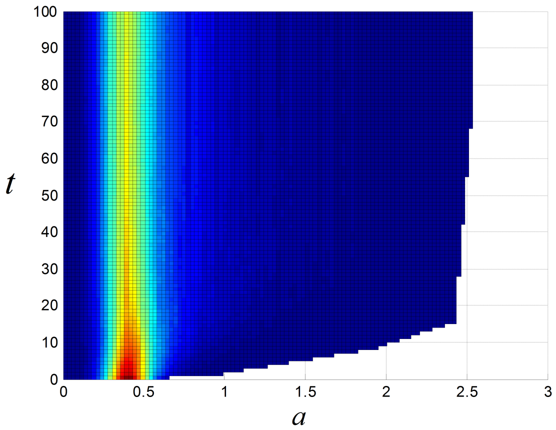
out that the total particle number N, average radius $\bar{a}$ and deviation of radius σ also fit exponential relation eq().

iv) Comparison and analysis:

Figures in section i)ii)iii) reveal one general characteristic that the system may start from different initial



(d)3D representation of $f(a,t)$



(e)contour of probability

FIG. 1: 3D representation of $f(a,t)$

TABLE I: fitting parameters

distribution	statistics	$y0$	A	τ
Gaussian	N	6374	33468	8.8
	$\bar{a}$	0.581	-0.185	15.85
	σ	0.352	-0.272	16.01
Uniform	N	6433	34350	12.85
	$\bar{a}$	0.589	-0.199	23.45
	σ	0.315	-0.279	21.64

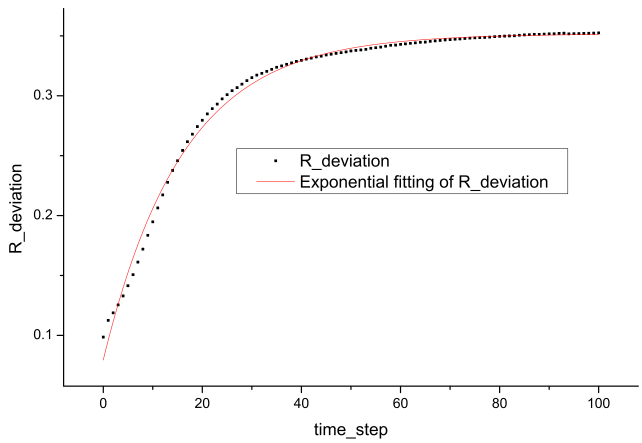
distributions but results in similar behaviour—$N(t), \bar{a}(t)$ and $\sigma(t)$ obey the same exponential form eq(), which means

$$\frac{d(N-N_0)}{dt} \propto (N-N_0) \tag{24}$$

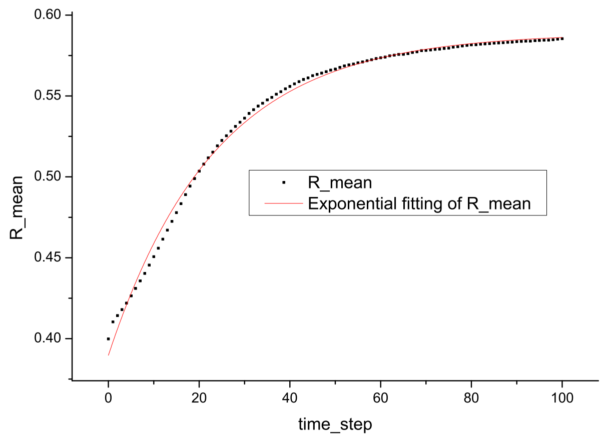
$$\frac{d(\bar{a}-\bar{a}_0)}{dt} \propto -(\bar{a}-\bar{a}_0) \tag{25}$$

$$\frac{d(\sigma_{-}\sigma_0)}{dt} \propto -(\sigma-\sigma_0) \tag{26}$$

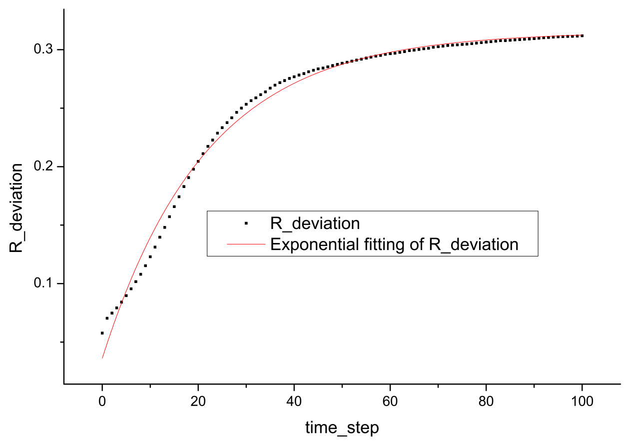
There's no surprise that equation (24) and equation (25



(a)exponential fitting of N

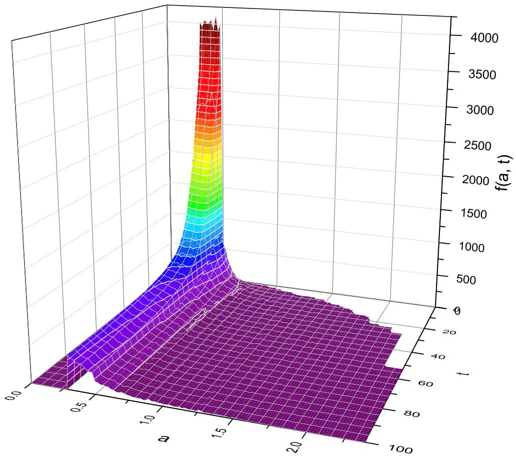


(b)exponential fitting of $\bar{a}$

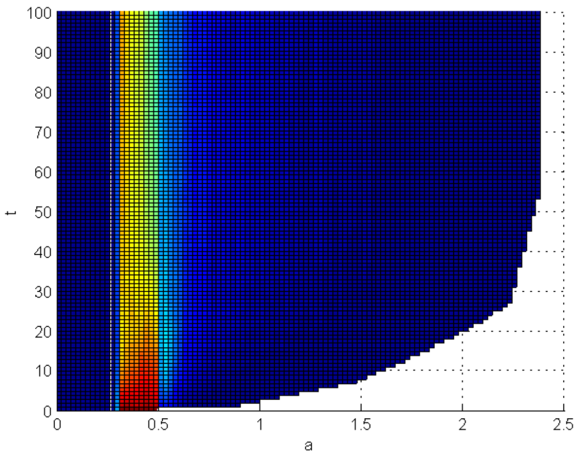


(c)exponential fitting of σ

will be roughly true. The left side of equation (24) represents the collision rate, which should be approximately proportional to the difference between the current bubble number and the asymptotic number, as more bubbles, more possibility to collide. Since the total volume is con-



(d)3D representation of $f(a,t)$



(e)contour of probability

FIG. 2: 3D representation of $f(a,t)$

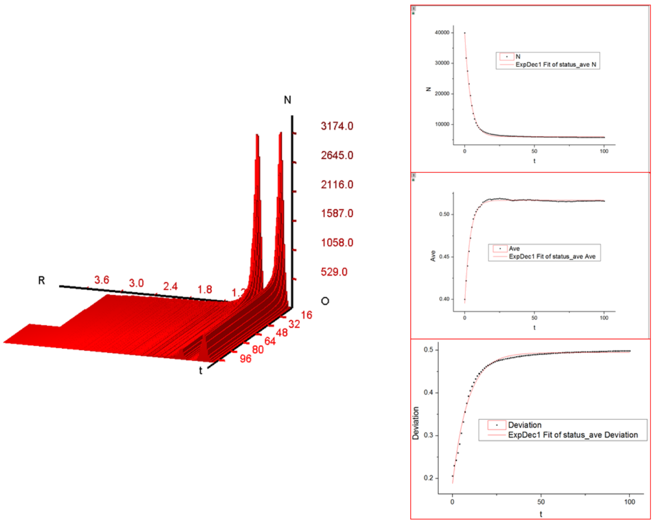


FIG. 3: two Gaussians

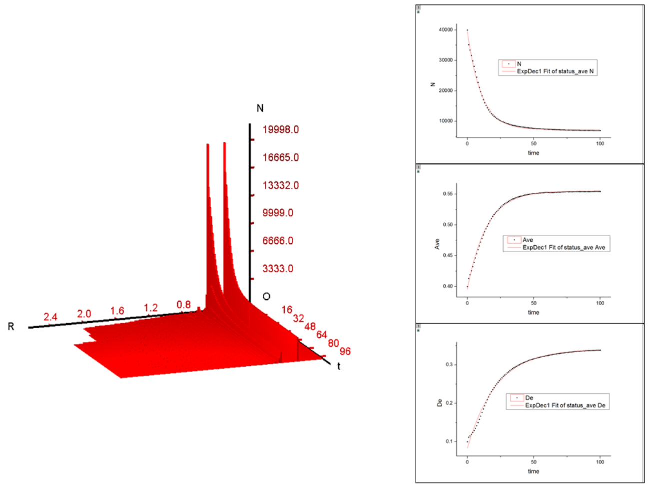


FIG. 4: two Deltas

served, the average radius is roughly

$$\bar{a}(t) \approx \bar{V}(t)^{1/3} = (V_{total}/N(t))^{1/3}$$

$$= [V_{total}/(N_0 + A_N e^{-t/\tau_N})]^{1/3}$$

further transformation shows that

$$\frac{d(\bar{a} - \bar{a}_\infty)}{dt} / (\bar{a} - \bar{a}_\infty) = \frac{\bar{a} - \bar{a}^4/\bar{a}_\infty^3}{\bar{a} - \bar{a}_\infty}$$

is almost a constant(varies slowly), so equation (25 is also statistically correct. The deviation $\sigma(t)$, actually doesn't fit the exponential form exactly, especially the beginning part. The quantitative explanation needs more dedicated work, but qualitatively speaking, number of big bubbles are always increasing, while some small bubbles never collides, causing the deviation larger and larger. The increasing rate should roughly be proportion to the collision rate, i.e. $N - N_0$. Hereby, it's plausible that $\sigma(t)$ has similar behaviour as $N(t)$, but with a negative coefficient A in eq()

Checking the fitting parameters in TABLE I, we can see that though the system starts from two kinds of distributions, the evolution coefficient $y0$ and A have minor differences, while σ, characteristic of the evolution rate, turn out to be quite different. It indicates that the system tends to evolute towards the same statistical average state regardless of the initial distributions, which only affects the reacting speed. Spontaneously, we expect that there're common features of the final asymptotic distributions.

When comparing the asymptotic function $f(a,\infty)$, we found that the tail parts are always roughly the same. It's better to illustrate how the tails merges with each other by a vivid animation of comparing Gaussian and uniform systems(accessible at URL1), and figure 5 and 6 are two snapshots at t=0, and t=100(100-steps is treated as the step unit).

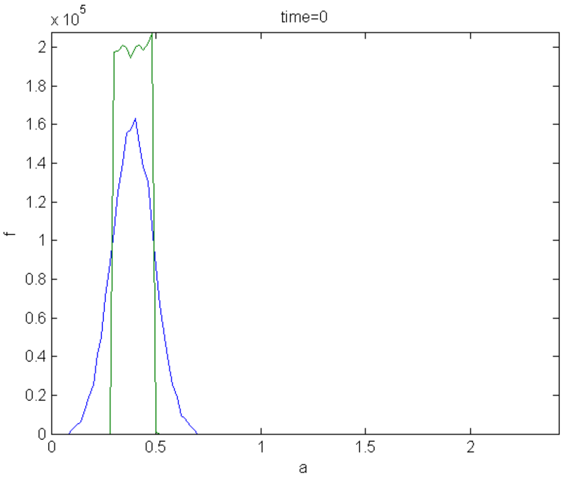


FIG. 5: t=0

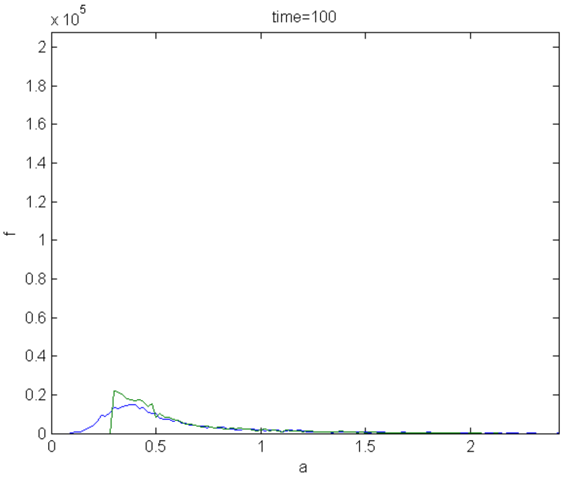


FIG. 6: t=100

The integration of the difference between two systems can be defined as

$$I(t) = \int_0^\infty [f_1(a,t) - f_2(a,t)]^2 da \tag{27}$$

which represents the overall difference and decays with time as shown in figure (7), indicating that systems indeed get closer and closer as we expected. By plotting $[f_1(a,\infty) - f_2(a,\infty)]^2$ in figure (), we can better determine where's the starting point a^* of the common tail. Then we can isolate the tail part data and do nonlinear fittings. After many trials, it turns out that the Hill 1 form, which is originally used to describe chemical reaction, fits best for the tail

$$y = start + (end - start)\frac{x^n}{k^n + x^n} \tag{28}$$

as shown in figure (9). Is the Hill form an accident or resulting from some hidden relation? More study is called here. But we do find a simple form to describe the common asymptotic part.

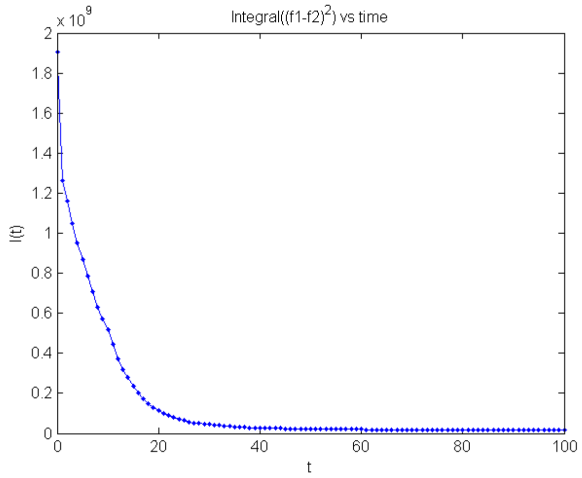


FIG. 7: I(t)

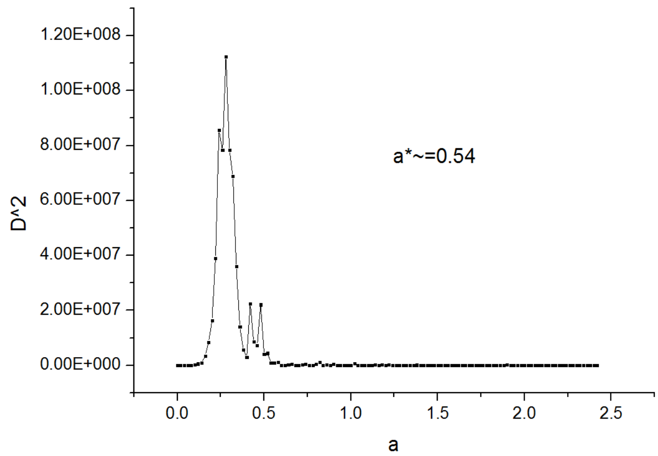


FIG. 8: D^2

v) Examine the modified Smoluchowski equation In last section, we developed an evolution equation (19) based on Smoluchowski equation. Let's use the numerical results generated by molecular dynamics simulation to examine the correctness of our theory. Equation (19) is written in distribution function $g(V,t)$ of volume V while in real simulation, it's more convenient to obtain distribution function in terms of radius a. Due to conservation of particles, we get a simple translation:

$$g(V,t)dV = f(a,t)da \Rightarrow g(V,t) = \frac{3}{4\pi} f(a,t)/a^2 \tag{29}$$

To simply the test, we only consider the final asymptotic balanced state, where $\frac{\partial f(V,t)}{\partial t} = 0$, so that theoreti-

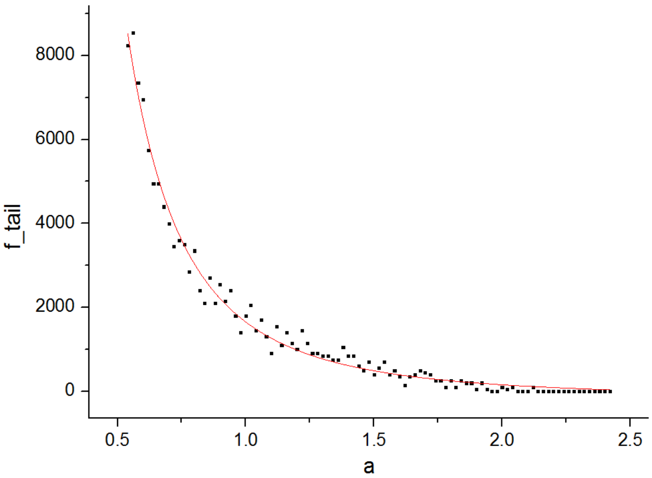


FIG. 9: f_{tail}

cally the bubbles forming rate should be equal to breaking rate,i.e.

$$\int_{V/2}^{V} dV' g(V') g(V-V') [V'^{1/3} + (V-V')^{1/3}][V'^{2/3} - (V-V'$$

$$= \int_{0}^{V} dV' g(V') g(V) (V'^{1/3} + V^{1/3})(V'^{2/3} - V^{2/3}) \quad (30)$$

Let's use the simulation data for Gaussian distribution to calculate R_{form} and R_{break}(R means rate), as shown in figure (10),

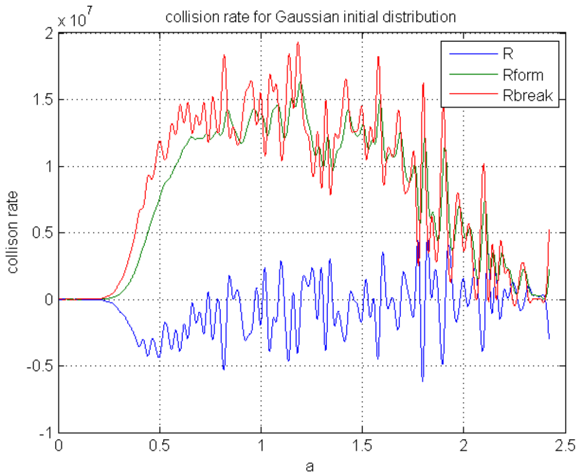


FIG. 10: R by original data

We can see that R_{form} and R_{break} are almost balanced if averaging the noise. More careful observation reveals that the oscillations of R_{form} and R_{break} have same tendency but with minor lag. Spontaneously, we

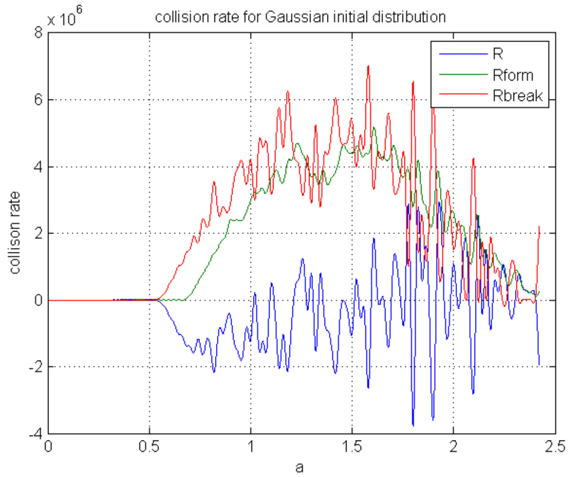


FIG. 11: R by tail part of original data

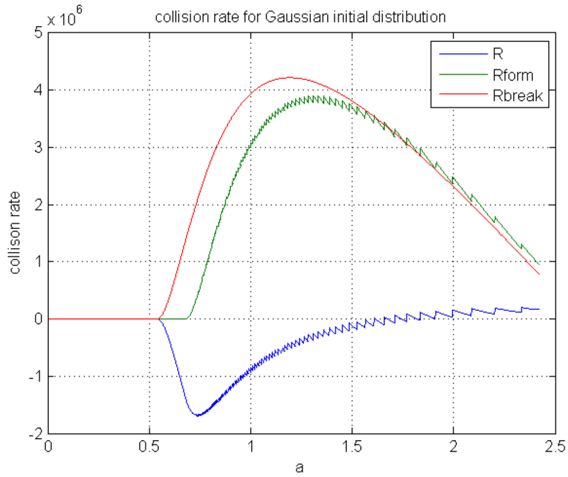


FIG. 12: R by tail part from Hill function

wonder if the beginning part has a significant effect on $R_{form} - Rbreak$. Then we only plug the tail into eq(30), and redraw collision rates in figure (11), which demonstrates a similar behavior as figure(10) and a little bigger lag between two rates. It means that the tail, a common part regardless of the initial distribution, is the leading part that determines the balance of the asymptotic state. Finally, let's test the fitting Hill 1 function in equation (30), which turn out to be much smoother as shown in figure (12). Since we leave out the beginning part, it's natural that $R_{form} - Rbreak$ is not well balanced around the cutting edge, but becomes better in for large a.

Above analysis showed that our simulation data is, to certain extent, consistent with the theoretic equation (19), especially the tail part generated during the evolution. Note equation (19) is developed based on a space-uniform assumption, which is only approximately true in our system. As more precise theory considering space as a variable makes the math quite messy, equation (19) turns out to be a good and elegant approximation in such a directed coagulation problem.

vi) Summary of the simulation

a)The total bubble number $N(t)$, average radius $\bar{a}(t)$ and deviation of radius $\sigma(t)$ roughly obey exponential form $y = y_0 + Ae^{-t/\tau}$,.

b)Initial distribution mainly affects how fast the system evolves to the asymptotic one, i.e. parameter τ.

c)The asymptotic distributions shares the same tail, but the beginning of the tail may be different. The tail can be approximately described by Hill 1 function $y = start + (end - start)\frac{x^n}{k^n+x^n}$

/***/

VI. The case of Sticking Bubbles.

The problem of colliding bubbles which stick to each other but do not merge is qualitatively similar to the one discussed above. We also have analogous, partial mergers where companies pool together their resources maintaining some individuality within an overall umbrella framework . We will not follow this analogy and focus on the bubbles case perse.

The sticking bubbles form conglamorates of adjacent bubbles or "Supper-Bubbles" with an effective radius R. The total volume V of the individual bubbles in the super-bubble is :

$$V = \frac{4\pi d R^3}{3}. \tag{31}$$

with the dilution factor $d < 1$ accounting for spaces between quartets of adjacent spheres. In two dimensions, the regions between triplets of tangent circular bubbles are disconnected. I the three dimensional case of interest the iter-bubble regions along with the rest of the fluid , form one connected domain . This allows in addition to external flow around the outside surface of the super-bubble also "internal" flow between the above interstitial holes. Intuitively we expect that the internal, torturous paths offer much stronger (viscous) resistance and the liquid displaced by the upward motio n of the s-bubble flows mainly outside,around the external contour of the s-bubble approximated by a sphere of radius R .

We expect a resultant "Stokes" like drag

$$F_D \approx 6\pi\eta v R. \tag{32}$$

The buoyant force , just like in the previous case of complete merge, is proportional to the total net bubble volume - namely to V of Eq.(31) above. The analog of the principle of minimal action for conservative systems-is minimal dissipation for frictional systems. In the present context this principle dictates minimal internal flow and smoothing out of the external flow on the scale of the roughness of the external surface of the $s-$bubble. To the extent that the roughness scale is smaller than the effective radius $R-$ this justifies then Eq.(32).

VII. Application

This process of directed coagulation is not limited to bubbles, but also applicable for many phenomenon in the nature, such as the formation of rain drops, bacterial swarms, animal flock, commercial operations, etc, all of which roughly obey the statistical results we list. We can predict the number, the average size, and the deviation evolving with time, and the asymptotic form of the distribution. Or on the contrary, get the properties of initial distribution, which is usually unknown, by measuring the later form.

[1] L. D. Landau, E. M. Lifshitz, and L. P. Pitaevskii, *Electrodynamics of Continuous Media*, Vol. 8 (Butterworth-Heinemann, Oxford, 1996).

[2] Antoine Bricard, Jean-Baptiste Caussin, Nicolas Desreumaux, Olivier Dauchot, Denis Bartolo, *Emergence of macroscopic directed motion in popula- tions of motile colloids*

[3] P. Cremer, H. Lowen, *Scaling of cluster growth for coagulating active particles*

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[5] Joseph D. Paulsen, *The Approach and Coalescence of Liquid Drops in Air*

[6] M. K. Zhekamukhov, B. G. Karov, and T. S. Kumykov, *Electrization and Spatial Charge Separation at the Air Bubbles Exhalation That Occurs During the Coagulation Growth of Hail Particles in a Cloud*