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Solutions to the mean-field equations of branchless diffusion-limited aggregation

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A problem with the *quasistatic* mean-field equations for branchless diffusion-limited aggregation, which were given and solved by Cates [Phys. Rev. A **34**, 5007 (1986)], is pointed out and resolved. In particular, it is shown that the exponent γ describing the time dependence of the growing aggregate (which was set infinite by Cates) equals $\frac{1}{2}$ on the mean-field level. An approximate analytical solution to the *full* mean-field equations is presented and compared with its numerically exact counterpart. Properties of the aggregate boundary as described by the exact solution are derived analytically. It is shown that scaling of the aggregate density *at all times* implies that the random-walker density cannot satisfy simple constant (nonzero) density or flux boundary conditions at infinity.

Since the invention of the Witten-Sander model[1] for diffusion-limited aggregation (DLA) it has become clear that, despite their simplicity in conception, nontrivial analytical statements about growth models of this kind are not easily obtained. To supplement the few available rigorous[2] or "almost" exact[3] results with further information, one has to have recourse to rather strong approximations, such as mean-field equations for continuous density versions of the model,[4] shape hypotheses,[5,6] or simplifications of the model itself.[7,8]

One of these simplifications is branchless DLA,[7] where growth proceeds by aggregation of diffusing particles at the tips of existing clusters only. Thus the ensuing aggregate is a forest of growing needles. The model neglects one of the aspects leading to the tenuous structure of DLA—branching—but exhibits in detail another—the competition of growing "trees" for the incoming random walkers and the accompanying growth instability. Nontrivial scaling was found in numerical simulations.[7,9]

Recently, an exact solution to the quasistatic version of the mean-field equations for branchless DLA on a flat substrate was reported by Cates.[10] The purpose of this Comment is to point out and remedy a deficiency of this approach. In the course, the arbitrariness regarding the definition of time that is implicit in Cates's analysis and kept one of the scaling exponents indeterminate will be removed, allowing its calculation. An approximate solution preserving some features of the one presented by Cates and an exact scaling solution are given. These two solutions essentially exhaust the generic behavior of all physical solutions exhibiting a scaling aggregate *density*, which allows certain conclusions regarding the boundary conditions needed to obtain scaling.

The equations to be discussed are

$$\frac{\partial\rho}{\partial t}=-u\frac{\partial\rho}{\partial r}\ , \qquad (1a)$$

$$\frac{\partial\rho}{\partial t}+\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial r^2}\ . \qquad (1b)$$

Herein, the density $\rho(r,t)$ of the aggregate is proportional to the number of needles having heights greater than r at time t. $u(r,t)$ is the density of random walkers. Time t and coordinate r have been appropriately rescaled so as to make the absorption rate factor in (1a) as well as the diffusion constant in (1b) equal to 1. Equation (1a) becomes obvious as soon as one realizes that the density of absorbing needle tips ρ_{tip} is given by[10] $\rho_{\text{tip}}=-\partial\rho/\partial r$. Equation (1b) is just the continuity equation. As usual, Cates neglects $\partial u/\partial t$, thus introducing a quasistatic limit.[10] He then derives a piecewise exact solution of these equations via a scaling ansatz $\rho(r,t)=r^{-\alpha}f(r/e^{\mu t})$ with $\alpha=1$:

$$\rho(r,t)=2[r^{-1}-\xi^{-1}(t)],\quad r\le\xi(t) \qquad (2a)$$

$$u(r,t)=\mu r^2\xi^{-1}(t),\quad r\le\xi(t) \qquad (2b)$$

$$\rho(r,t)=0,\quad r\ge\xi(t) \qquad (2c)$$

$$u(r,t)=\mu[2r-\xi(t)],\quad r\ge\xi(t) \qquad (2d)$$

where $\xi(t)=e^{\mu t}/\lambda$. μ (>0) is fixed by the boundary condition at infinity $[\mu=\frac{1}{2}(\partial u/\partial r)|_{r=\infty}]$, λ by the value of $\xi(0)$.

Let us now calculate $\partial\rho/\partial t$ and $\partial u/\partial t$ at the maximum needle height $\xi(t)(-0)$. From the result $\partial\rho/\partial t=2\mu\xi^{-1}(t)$, $\partial u/\partial t=-\mu^2\xi(t)$ we conclude that $|\partial\rho/\partial t|\ll|\partial u/\partial t|$ after times larger than $t'=\ln(2\lambda^2/\mu)/2\mu$. Therefore $\partial u/\partial t$ is not generally negligible in (1b). Even if the time t', up to which it *can* be neglected for $r \le \xi(t)$, is *large* (because μ is small or λ large), $\partial u/\partial t$ should *not* be considered negligible *at all* for $r > \xi(t)$, where $\partial \rho/\partial t = 0$. In short, the quasistatic limit becomes inaccurate in that region.

Consider now the (generalized) scaling ansatz $\rho(r,t) = \rho_0 + r^{-\alpha} f(r/t^\gamma)$. Denoting the scaling variable r/t^γ by x, we have $\partial\rho/\partial t = r^{-\alpha-1/\gamma} f_1(x)$, $\partial\rho/\partial r = r^{-\alpha-1} f_2(x)$, which together with (1a) implies

$$u = r^{1-1/\gamma} g(x), \quad \partial u/\partial t = r^{1-2/\gamma} g_1(x) ,$$

$$\partial^2 u/\partial r^2 = r^{-1-1/\gamma} g_3(x) .$$

Insertion into (1b) leads to

$$r^{-\alpha-1/\gamma} f_1(x) + r^{1-2/\gamma} g_1(x) = r^{-1-1/\gamma} g_3(x) . \tag{3}$$

From (3) we immediately obtain the exponents $\alpha = 1$, $\gamma = \frac{1}{2}$. Note that by neglecting the second term on the left-hand side of (3), which is $\partial u/\partial t$, one renders γ indeterminate. This corresponds to the arbitrariness in the definition of time as stated by Cates,[10] who then chose $\gamma = \infty$ in order to obtain constant flux boundary conditions. Once the $g_1(x)$ term in (3) is neglected, the set of (nonlinear) differential equations for the scaling functions following from (3) can be solved for arbitrary γ (see below).

Introducing $F(x) = x^{-1} f(x)$ and $G(x) = x^{1-1/\gamma} g(x)$ [hence $\rho(r,t) = \rho_0 + t^{-\gamma} F(x)$, $u(r,t) = t^{\gamma-1} G(x)$] we obtain a set of ordinary differential equations:

$$[G(x) - \gamma x] F'(x) = \gamma F(x) , \tag{4a}$$

$$\gamma \frac{d}{dx} x F(x) = -G''(x) - \gamma \frac{d}{dx} x^{1/\gamma - 1} G(x) . \tag{4b}$$

Neglecting $\partial u/\partial t$ in (1b) would now correspond to dropping the $G(x)$ term in (4b). A solution can then be found that is formally very similar to the one given in Ref. 10:

$$F(x) = \frac{2}{x} - 2\lambda, \quad G(x) = \gamma\lambda x^2, \quad x \le \frac{1}{\lambda} \tag{5a}$$

$$F(x) = 0, \quad G(x) = 2\gamma x - \frac{\gamma}{\lambda}, \quad x \ge \frac{1}{\lambda} . \tag{5b}$$

Introducing the aggregate height $\xi(t) = t^\gamma/\lambda$ and computing again $\partial\rho/\partial t$ and $\partial u/\partial t$, we find

$$\frac{\partial u}{\partial t}(\xi(t)-0, t) = -\gamma(\gamma+1)\frac{1}{\lambda} t^{\gamma-2} , \tag{6a}$$

$$\frac{\partial \rho}{\partial t}(\xi(t)-0, t) = 2\gamma\lambda t^{-\gamma-1} , \tag{6b}$$

which shows that $\gamma = \frac{1}{2}$ is a marginal exponent: for larger values of γ, $\partial u/\partial t$ is not negligible inside the aggregate in comparison with $\partial\rho/\partial t$; for $\gamma = \frac{1}{2}$, $\partial u/\partial t$ is negligible at all times, if only λ is large enough; for smaller γ values, $\partial u/\partial t$ is always asymptotically negligible.

Hence, for $\gamma = \frac{1}{2}$, Eq. (5a) together with the scaling ansatz qualifies as an *approximate* solution to the *full* mean-field equations *inside* the aggregate. However, Eq. (5b)—predicting $u(r,t) \to \infty$ for $r \to \infty$—is not even qualitatively correct *outside* the aggregate, as will be seen in the following. Equations (4) may be rewritten as a set of integral equations, which for $\gamma = \frac{1}{2}$, read

$$F(x) = a \exp\left[\int_{x_1}^{x} dz \frac{1}{2G(z) - z}\right] , \tag{7a}$$

$$G(x) = b \exp[-\tfrac{1}{4}(x^2 - x_2^2)] + \int_{x_2}^{x} dz \exp[-\tfrac{1}{4}(x^2 - z^2)][c - \tfrac{1}{2} z F(z)] , \tag{7b}$$

where a, b, and c are constants of integration.

Since $F(x) \equiv 0$ solves the first of these equations, the second provides an explicit solution in this case. Imposing continuity and differentiability at $x = 1/\lambda$, we can match the exact solution for $x \ge 1/\lambda$ to the approximate one for $x \le 1/\lambda$ and get

$$G(x) = \frac{1}{2\lambda} \exp\left[-\frac{1}{4}\left[x^2 - \frac{1}{\lambda^2}\right]\right] + \left[1 + \frac{1}{4\lambda^2}\right] \int_{1/\lambda}^{x} dz \exp[-\tfrac{1}{4}(x^2 - z^2)] . \tag{8}$$

Using (5a) and (8), we find that a decent approximation to a scaling solution of Eqs. (1) should be given by

$$\rho(r,t) = \rho_0 + 2[r^{-1} - \xi^{-1}(t)], \quad r \le \xi(t) \tag{9a}$$

$$u(r,t) = \tfrac{1}{2} r^2 t^{-1} \xi^{-1}(t), \quad r \le \xi(t) \tag{9b}$$

$$\rho(r,t) = \rho_0, \quad r \ge \xi(t) \tag{9c}$$

$$u(r,t) = \left[t^{-1} + \left[\frac{\xi(t)}{2t}\right]^2\right] \int_{\xi(t)}^{r} dz \exp\left[-\frac{1}{4t}(r^2 - z^2)\right] + \frac{\xi(t)}{2t} \exp\left[-\frac{1}{4t}[r^2 - \xi(t)^2]\right], \quad r \ge \xi(t) \tag{9d}$$

where $\xi(t) = t^{1/2}/\lambda$. Figure 1 displays this solution for several finite times and at $t = \infty$. To assess its quality, the scaling functions are compared with numerically exact solutions of the system (4) in Figs. 2 and 3. The boundary conditions have been chosen such that the solution coincides with (5a) at a small positive value $x = \epsilon$ [i.e., $x_1 = x_2 = \epsilon$, $a = 2/\epsilon - 2\lambda$, $b = \frac{1}{2}\lambda\epsilon^2$, and $c = 1 + \frac{1}{4}\lambda\epsilon^3$ in (7)]. Comparison of Figs. (2a) and (2b) shows that the agreement between approximate and exact solutions improves with increasing λ, as anticipated, and is already very good for $\lambda = 2$. Even for $\lambda = 1$, an appreciable difference between the aggregate densities of the exact and the approximate solutions appears only close to the interface separating the regions with and without aggregate. The solution (9) tends to the exact infinite time limit $\rho(r,t) = \rho_0 + 2/r$, $u(r,t) = 0$ [Eqs. (4) are solved exactly by $F(x) = A/x$, $G(x) \equiv 0$]. Comparing (2) with (9) we see that the former result provides quite an acceptable representation of the *spatial* dependence of the *aggregate* density (but not of its time dependence) and even correctly reproduces the infinite time limit. However, if a solution is to ever become a reasonable starting point of a perturbative expansion in a noise term,[11] it should also well approximate the *diffusion* field, which is only done by the new solution.

The exact solution to the full mean-field equations

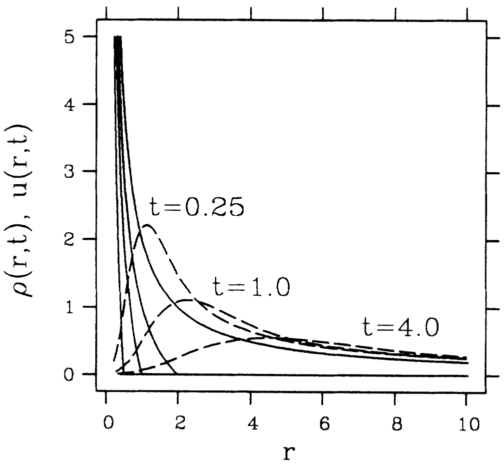

FIG. 1. Aggregate density ρ and random-walker density u as a function of height r for several times t, according to the approximate solution (9), with $\xi(1)=1$. Solid lines, $\rho(r,t)$; dashed lines, $u(r,t)$. The cases $t=0.25$, 1.0, 4.0, and ∞ are displayed [in the plot, $u(r,\infty)\equiv 0$ is not distinguishable].

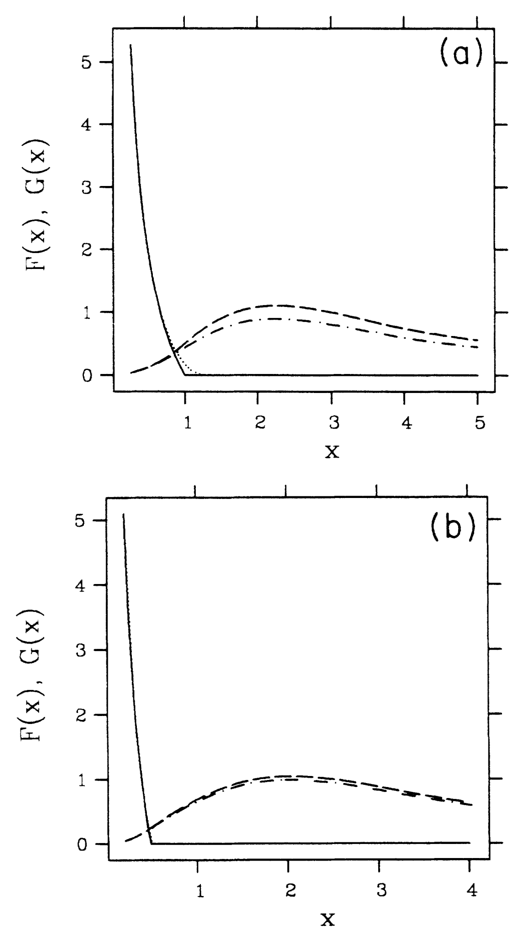

FIG. 2. (a) Scaling functions $F(x)$ and $G(x)$; comparison of the approximate solution with the exact solution for $\lambda=1$. Solid line, $F(x)$ according to (5a) and (5b); dashed line, $G(x)$ according to (5a) and (8); dotted line, (numerically) exact $F(x)$, $F(x)\equiv 0$ beyond $x_0 \approx \sqrt{2}$; dash-dotted line, exact $G(x)$. (b) Same for $\lambda=2$. Solid and dashed lines, approximate solutions for $F(x)$ and $G(x)$; dotted and dash-dotted lines, exact solutions.

differs from the approximate one in some respects that can be investigated analytically. First note that if $G(x)$ remains smaller than $\frac{1}{2}x$ for all $x>0$, $F(x)$ never actually becomes zero, i.e., the aggregate boundary is not sharp. This situation occurs whenever $\lambda<\lambda_c$ (Fig. 3); the numerical results suggest that the critical value is $\lambda_c=1$. For $\lambda<\lambda_c$, Eqs. (9) are not a good approximation. If $\lambda=\lambda_c$, the graph of $G(x)$ touches the line $y(x)=\frac{1}{2}x$, say at x_0. Then it follows from $G(x)=\frac{1}{2}x-(1/2\bar{\beta})(x-x_0)^2$ for $x\approx x_0$ that $F(x)\sim\exp[-\bar{\beta}/(x_0-x)]$ for $x\to x_0-0$ [see (7a)], meaning that $F(x)$ has an *essential singularity* at x_0 and actually takes on the value zero there. Obviously, the solution can be continued as $F(x)\equiv 0$ for $x>x_0$, and all derivatives remain continuous at x_0. For $\lambda>\lambda_c$, $G(x)$ has (two) intersection points with $y=\frac{1}{2}x$. Let x_0 be the smallest abscissa of these points and $G(x)=\frac{1}{2}x+(1/2\beta)(x-x_0)$ for $x\approx x_0$. Then, because of (7a), $F(x)\sim(x_0-x)^{\beta}$ for $x\to x_0-0$. Furthermore, it can be shown that, for $\epsilon\to 0$, x_0 and β are related to each other via

$$x_0^2=2-\frac{2}{\beta}\ . \tag{10}$$

This equation demonstrates that for this possibility to be realized (which it is as the numerics shows) β has to exceed 1 (which is difficult to see in the numerical solution). Therefore $F'(x)$ exists and is zero at $x=x_0$, and $G''(x)$ is also continuous there. Because the solution is then continued as $F(x)\equiv 0$ for $x>x_0$, the second intersection of $G(x)$ with $y=\frac{1}{2}x$ does not play any role. At $\lambda=\lambda_c, x_0=\sqrt{2}$, which is the maximum value attainable; as λ increases, the relation $x_0=1/\lambda$ becomes an improving approximation. Note that for the *approximate* solution λ is a fundamental quantity, determining the interface position. In the *exact* solution, however, it merely describes the asymptotic behavior of $F(x)$ as $x\to 0$, while it is the parameter x_0 which determines the *location* as well as the *analytic structure* of the interface.

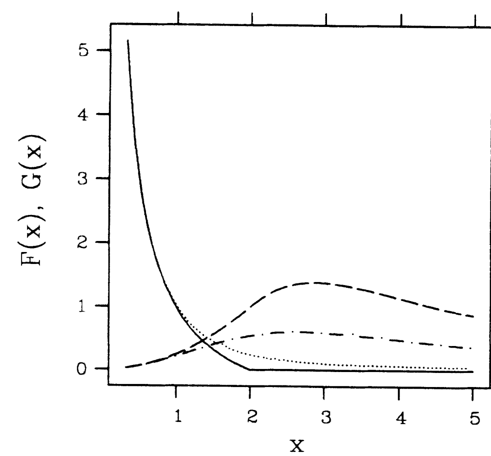

FIG. 3. Comparison of the approximate scaling functions $F(x)$ and $G(x)$ with their exact counterparts for $\lambda=\frac{1}{2}$. The exact solution $F(x)$ never meets the x axis.

To summarize, the solutions constructed to agree with (5a) for $x \to 0$ fall into two classes. For $\lambda < \lambda_c$, there is no (sharp) aggregate boundary, i.e., x_0 does not exist. These solutions correspond to a situation where arbitrarily high needles are already present in the initial aggregate—a case that is not considered in simulations. For $\lambda > \lambda_c$ an interface exists at x_0. Contrary to what is suggested by the approximate solution (9), the aggregate density does not rise sharply with a finite slope there, but increases smoothly in the way discussed above.

If instead of $F(\epsilon)=2/\epsilon-2\lambda$, one requires $F(\epsilon)=A/\epsilon-2\lambda$ [motivated by the existence of an exact solution with $F(x)=A/x$], the situation is a little different. Equation (10) is then replaced with $x_0^2=2A-2-2/\beta$, which for $A>2$ allows solutions with $\beta \leq 1$. These solutions actually cross the x axis at x_0 and continuing them by $F(x)\equiv 0$ would render $F'(x)$ discontinuous. For $A<2$, the foregoing discussion still applies, but the maximum value for x_0 is decreased and the minimum value for β increased. For $A \leq 1$, there are only solutions with a diffuse interface.

As $r \to \infty$, $u(r,t)$ goes to zero or, equivalently, $\lim_{x\to\infty} G(x)=0$. It can be shown rigorously that this property holds for all solutions with $F(x) \geq 0$ and $G(x) < \frac{1}{2}x$ initially. This means that there is *no physical scaling solution* with $\rho_0=0$ that satisfies simple, i.e., either constant density ($\neq 0$) or constant flux boundary conditions at infinity.

However, our generalized scaling ansatz admits the possibility of *negative* $F(x)$ as long as $\rho_0 t^{1/2} > -F(x)$. An exact solution to (4) (with $\gamma=\frac{1}{2}$) is

$$F(x)=-x, \quad G(x)=x , \tag{11}$$

leading to

$$\rho(r,t)=\rho_0-\frac{r}{t}, \quad u(r,t)=\frac{r}{t} . \tag{12}$$

Because the result for $\rho(r,t)$ is not bounded from below, it can represent a physical solution to (1) in a limited space-time domain at best. In particular, the description becomes invalid for $r \to \infty$. Equation (12) might describe a finite system into which a constant particle flux is fed from one side, or else a transient scaling state (in a finite domain) of an essentially nonscaling solution of (1). Therefore also this somewhat pathologic solution does not allow for simple boundary conditions. It is asymptotically stable, and all negative solutions with $F'(x)<0$ and $G(x)>\frac{1}{2}x$ converge to it, unless $G(x)$ manages to cross the line $y=\frac{1}{2}x$, in which case $F(x) \to 0$ and $G(x) \to 0$ for $x \to \infty$.

Hence, for positive physical solutions [which have $F'(x)<0$] the density of random walkers decays to zero at infinity, while negative solutions become unphysical at large r. Only for special initial distributions of walkers (given at a time slightly larger than $t=0$), can one expect scaling behavior. This seems at odds with numerical simulations which show (nontrivial) density scaling until a single needle survives. The reason is presumably that simulations of the model operate in the zero-density limit—a new random walker is started only after the last one has aggregated. This limit is not well represented for *all times* by the mean-field equations (1). Rather one would have to consider a sequence of mean-field descriptions with decreasing initial densities $u(r,t_0)$ at increasing aggregate sizes. In the simulation of a *finite-density system* with $u(r,t)$ approaching a constant value at infinity, one would expect that at large times, a stationary state evolves which consists of an array of needles separated by roughly the diffusion length l and growing at constant velocity and constant density $\sim 1/l^{d-1}$. This means that the *density* would no longer scale. However, the *height* $\xi(t)$ of the aggregate would scale as $\xi(t) \sim t$ and should, if there is a region of density scaling, show a crossover from an exponent $\gamma<1$ ($\frac{1}{2}$ in mean-field approximation) at small times to $\gamma=1$ at large times. In the light of these considerations, it seems interesting to simulate the branchless model with finite walker densities to find out, to what extent scaling properties survive under, e.g., constant density boundary conditions.

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