SELF-SIMILAR BLOWUP SOLUTIONS TO AN AGGREGATION EQUATION IN R^{n*}

YANGHONG HUANG[†] AND ANDREA L. BERTOZZI[†]

Abstract. We present numerical simulations of radially symmetric finite time blowup for the aggregation equation $u_t = \nabla \cdot (u \nabla K * u)$, where the kernel $K(x) = |x|$. The dynamics of the blowup exhibits self-similar behavior in which zero mass concentrates at the core at the blowup time. Computations are performed in R^n for n between 2 and 10 using a method based on characteristics. In all cases studied, the self-similarity exhibits second-kind (anomalous) scaling.

1. Introduction. In this paper, we consider the self-similar blowup of radially symmetric solutions to the aggregation equation

$$(1.1) \qquad u_t = \nabla \cdot (u \nabla K * u) \quad \text{in } [0, T) \times \mathbb{R}^n,$$

subject to initial condition $u(0, x) = u_0(x)$ on some time interval of existence $[0, T)$. Here $K * u$ is the convolution of u with a radially symmetric kernel potential K. This equation arises in a number of continuum models for interacting particles via pairwise potentials. It appears in the description of self-assembly of nanoparticles by Holm and Putkaradze [32, 33] as an alternative to the Debye–Huckel or Keller–Segel model. It is also used as a popular model for aggregation in animal behavior, e.g., the schools or swarms formed by fish and birds, where everyone senses the presence of other individuals [12, 19, 20, 44, 49, 48]. In these applications the most common potential in the literature is $K(x) = 1 - e^{-|x|}$, which behaves like $|x|$ near the origin. These are examples of Lipschitz continuous potentials for which the lack of higher regularity at $x = 0$ is known to be responsible for the finite time blowup.

The basic properties of (1.1), with a "pointy" potential as described above, have been addressed recently in a series of papers. Bodnar and Velazquez [12] study the problem of existence and uniqueness, along with blowup and steady states in one dimension for different potentials with smooth initial data. The local existence and uniqueness of this equation in higher dimensions is proved by Laurent [38]. An alternative local existence and finite time blowup proof is given by Bertozzi and Laurent in [8]. The blowup problem is revisited in [7] and the review article [9] with a more general class of potentials, for which it is determined that an Osgood condition on the regularity of the potential at the origin is necessary and sufficient for finite time blowup. Moreover, it is shown that there is no mass-concentrating, smooth self-similar finite time blowup solution in odd dimension larger than one for the homogeneous, radially symmetric kernel $K(x) = |x|$. This fact is the primary motivation for the

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study here—namely, that the most common multidimensional models in the literature are known to produce finite time singularities, and in some higher dimensions, no smooth similarity solutions exist that concentrate mass. The paper [7] has a simple example in one dimension of a mass-conserving similarity solution. In higher dimensions they show some interesting similarity solutions that concentrate mass, but all of these involve collapsing delta-rings and thus cannot result from smooth initial data. By performing numerical calculations with a high degree of spatial and temporal precision, we are able to resolve the dynamics of blowup for this problem in multiple space dimensions. Our assumption of radial symmetry allows us to obtain a degree of precision that would be much more difficult in the case of solutions lacking symmetry.

Finite time blowup phenomena appear in many equations for physical models, including semilinear heat equations [29, 28], nonlinear Schrödinger equations [30, 42, 27], gravitational collapse [14], and pinchoff in surface diffusion [5]. For a general review article, see [26]. Near the blowup time, it often happens that, because of the absence of any external scales, the solution collapses to the singularity in a self-similar way. Probably the most extensively studied one is the semilinear heat equation

$$(1.2) \qquad u_t = \Delta u + f(u), \qquad f(u) = u^p \text{ or } f(u) = e^u.$$

However, it has been well known since the 1970s that there is no exact self-similar solution of the form (for $f(u) = u^p$)

$$(1.3) \qquad u(x,t) = (T-t)^{-1/(p-1)} U(x/(T-t)^{1/2}).$$

A refined analysis or center manifold theory close to the blowup time gives the following asymptotic behavior with a logarithm correction [25, 28, 29, 43]:
(1.4)
$$u(x,t) \sim \left(\frac{\beta}{T-t} \right)^{\beta} \left(1 + \frac{p-1}{4p} \eta^2 \right), \quad \text{where } \eta = \frac{x}{\sqrt{[(T-t)|\ln(T-t)|]}}, \ \beta = \frac{1}{p-1}.$$

In contrast, quasi-linear problems [47, 16]

$$(1.5) \qquad u_t = (|u_x|^\sigma u_x)_x + e^u \quad \text{or} \quad u_t = (u^\sigma u_x)_x + u^p, \quad \sigma > 0,$$

or higher order parabolic equations [17]

$$(1.6) \qquad u_t = (-1)^{m+1} D_x^{2m} u + |u|^{p-1} u, \quad \text{or} \quad u_t = (-1)^{m+1} D_x^{2m} u + e^u$$

do possess exact self-similar blowup solutions, where D_x^{2m} is the $2m$th derivative with respect to x.

For those solutions with nontrivial blowup profiles, it is possible that the profiles match the exact analytical ones only near the core of the blowup point (or set), with deviation (though very small in magnitude) away from the core, sometimes called quasi-self-similar solutions. This is observed in the collapse of the cubic nonlinear Schrödinger equation, either for the Townes profile [24, 42, 45] or for the ring profile [27].

In finite blowup problems for density distributions, the dynamics could concentrate a finite amount of mass or zero mass in the core, even for different types of blowup solutions of the same equation, which conserves the total mass. One example is the Keller–Segel system of equations, which models overdamped gravitational interaction of a cloud of particles and chemotaxis in bacteria [37]:

$$\partial_t \rho = \Delta \rho - \nabla \cdot (\rho \nabla c),$$

$$(1.7) \qquad\qquad -\Delta c = \rho,$$

where ρ is the density of the cloud or the bacteria and c represents the gravitational potential or the density of the chemo-attractant. In spatial dimension greater than two, there are at least two types of blowup solutions. One is exactly self-similar, concentrating zero mass, and the other is like a Burgers shock, with finite mass in a ring converging to the origin [13].

For all of the similarity solutions considered above, the similarity variables and exponents characterizing the dynamics, especially those related to the spatial spread, can be determined a priori, either from a dimensional analysis of the problem or from the basic invariant scales of the equation, called *self-similar solutions of the first kind* or *complete similarity solutions*. However, other problems exist in which self-similar scaling exponents cannot be determined from dimensional analysis; these are the so-called *similarity solutions of the second kind* or *incomplete similarity solutions* [3]. Among the first few problems studied are the nonlinear filtration by Barenblatt and Sivashinskii [4], Vázquez and collaborators [36, 2], and Peletier [46] and the focusing problem of the porous medium equation [35, 1]. In physics, those exponents are said to be *anomalous*. Sometimes renormalization group theory originated from quantum field theory is applied to the above-mentioned problems to find self-similar solutions of the second kind [31].

The goal of this paper is to show numerical evidence that the aggregation equation (1.1) has a family of radially symmetric, smooth self-similar blowup solutions. Those solutions appear to be exactly self-similar, concentrating zero mass in the core and of the second kind. The rest of the paper is organized as follows. The equation for the blowup profiles is derived in section 2, together with numerical observations of the profiles and anomalous exponents in different space dimensions. In section 3 we present the numerical methods used to simulate the blowup dynamics and a numerical renormalization group method to find the exponents iteratively. Additional numerical results about the postprocessing of the data from the blowup dynamics and the blowup in different L^p norms are given in section 4. We end this paper with some further directions and open questions in section 5.

2. Self-similar solutions of the blowup dynamics.

2.1. General theory for the self-similar blowup profiles. We introduce the similarity variables y and τ,

$$(2.1) \qquad\qquad y = x(T-t)^{-\beta}, \quad \tau = -\ln(T-t),$$

and define a new function $U(y, \tau)$ such that

$$(2.2) \qquad\qquad U(y,\tau) = (T-t)^\alpha u(y(T-t)^\beta, T - e^{-\tau}),$$

where T is the blowup time, and α and β are exponents characterizing the singularity when the blowup time is approached. We call the blowup dynamics self-similar if the transformed function U converges to some steady state as $t \to T^-$, or equivalently $\tau \to \infty$ for some appropriate constants α and β. When (2.2) is substituted into the original evolution equation for u, a routine calculation gives

$$
\begin{aligned}
(T-t)^{-\alpha-1} &\left(\partial_\tau U + \alpha U + \beta y \cdot \nabla U\right) \\
(2.3) \quad = (T-t)^{(n-2)\beta-2\alpha} &\nabla_y \cdot \left(U(y,\tau)\nabla_y \int_{R^n} K\left((y-z)(T-t)^\beta\right) U(z,\tau)dz \right).
\end{aligned}
$$

Therefore, a self-similar solution exists only if we can take the factor $(T - t)^\beta$ out of the kernel K. Thus K must be homogeneous, i.e., $K(\lambda x) = \lambda^d K(x)$ for some constant d and any λ. If the function u is concentrated on a small region in space, say the origin, then the kernel K can often be approximated by the leading nonconstant part (K is determined up to a constant), which is homogeneous. For this reason, in the rest of this paper, we will concentrate on the case with

$$(2.4) \qquad K(x) = |x|,$$

which is an approximation to the popular kernel $K(x) = 1 - e^{-|x|}$, and it is exactly the leading order $|x|$ in an even more general kernel that leads to finite time blowup [8, 7]. Given this, the matching of the exponents of $(T - t)$ in (2.3) gives

$$(2.5) \qquad \alpha = (n - 1)\beta + 1,$$

and the equation for U is

$$(2.6) \qquad \partial_\tau U = \nabla \cdot (U \nabla K * U) - \alpha U - \beta y \cdot \nabla U.$$

Any exact self-similar profile U, if it exists, must satisfy the steady equation of (2.6), i.e.,

$$(2.7) \qquad \nabla \cdot (U \nabla K * U) - \alpha U - \beta y \cdot \nabla U = 0, \qquad \nabla U|_{y=0} = 0, \quad \lim_{|y| \to \infty} U(y) = 0,$$

where U has no explicit dependence on τ. To completely characterize the self-similar blowup dynamics, we need one extra condition to find the exponent β. Very often this kind of information can be readily obtained from a dimensional analysis or scale invariance of the underlying equation, such as the parabolic scaling $\beta = 1/2$ for the semilinear heat equation and nonlinear Schrödinger equation, or $\beta = 1/(2m)$ for higher order parabolic equations as those in (1.6). Here, if the similarity solution concentrates mass in the core of the blowup, then $\alpha = n\beta$ from mass conservation, and consequently $\beta = 1$. However, numerical simulation of the blowup dynamics shows that no mass is concentrated. In fact, it is proved analytically in [7] that there is no such radially symmetric, self-similar solution in odd dimension larger than one that concentrates mass. The argument is straightforward so we review it here. Taking $\alpha = n$, $\beta = 1$ in (2.7), we can integrate the equation in radial coordinate $r = |y|$:

$$nU + rU_r = \frac{1}{r^{n-1}} \partial_r [r^{n-1} U \partial_r (K * U)].$$

Multiplying both sides by r^{n-1} and integrating once again, we get

$$r^n U = r^{n-1} U \partial_r (K * U).$$

Assuming U is nonzero, we divide by $y^{n-1} U$ and integrate up again to get the final result,

$$(2.8) \qquad \frac{1}{2} r^2 + C = K * U.$$

Now we recognize that in odd dimension n larger than one, for the special case of $K = |x|$, applying repeated Laplacians to the right-hand side of (2.8) gives $\Delta^{(n-1)} K * U = c_n U$, whereas the left-hand side gives $\Delta^{(n-1)}(y^2 + C) = 0$. Hence we do not have

a nontrivial exact similarity solution of the first kind (conserving mass) in odd space dimension larger than one. A more rigorous analysis and derivation of this is discussed in Lagrangian coordinates in [7]. In particular, that paper considers more general measure-valued similarity solutions due to the fact that there are easily constructed examples that concentrate mass in finite time in general space dimensions, starting with initial data of the form of a delta-ring (support of the solution concentrated on the boundary of a sphere). However, here we consider solutions with U, a bounded function of space. Thus it is reasonable to look for similarity solutions of the second kind, for which α and β satisfy (2.5), which comes from the dimensional analysis of the dynamics, but may violate conservation of mass.

The nonlocal nature of the kernel $K * U$ presents a much more difficult problem, both analytically and numerically, compared to local problems such as those from nonlinear diffusion equations and nonlinear Schrödinger equations. The usual techniques used to tackle the equation for the self-similar profiles, like phase plane analysis and shooting methods, do not work here. Smooth self-similar blowup solutions in one dimension are considered by Bodnar and Velazquez [12] for different kernel potentials K. The technique used there is to introduce an auxiliary function

$$(2.9) \qquad \psi(x,t) = \int_{-\infty}^{x} u(z,t)dz.$$

Moreover, for the special kernel $K = |x|$ considered here, the transformation (2.9) turns (1.1) in one dimension into $\psi_t = \psi_x(2\psi - c)$ with $c = \psi(\infty, t) = \int_{-\infty}^{\infty} u_0(z)dz$, which is a constant. Another change of variable $\phi = c - 2\psi$ gives exactly the well-known inviscid Burgers equation $\phi_t + \phi\phi_x = 0$. For general initial condition, the finite time blowup of u is equivalent to the onset of shock of ϕ, with mass concentration and thus $\alpha = \beta = 1$ as considered in [7]. However, for positive, even initial condition (the analogue for the radially symmetric case in higher dimension), the blowup exhibits a different scaling. Let the self-similar blowup solution of ϕ be

$$(2.10) \qquad \phi(x,t) = (T-t)^{\beta-\alpha} f(x(T-t)^{-\beta}).$$

Here the exponents are chosen such that $u = -\phi_x/2$ has the same form as (2.2). Similarly, we have $\alpha = 1$ and the equation for the profile

$$(2.11) \qquad ff' + \beta yf' - (\beta - 1)f = 0.$$

Because of the L^∞-contraction of the solutions to the Burgers equation, β must be equal to or greater than one. If $\beta = 1$, the only nontrivial solution is $f(y) = -y$, corresponding to the previous case. Otherwise if $\beta > 1$, we are looking for a power series expansion of f near the origin, i.e.,

$$(2.12) \qquad f(y) = a_1 y + a_3 y^3 + a_5 y^5 + \cdots.$$

The system of equations the coefficients must satisfy is

$$
\begin{aligned}
a_1^2 + a_1 &= 0, & O(y) \\
4a_1 a_3 + (2\beta + 1)a_3 &= 0, & O(y^3) \\
6a_1 a_5 + 3a_3^2 + (4\beta + 1)a_5 &= 0, & O(y^5)
\end{aligned}
$$

$$(2.13) \qquad \vdots$$

If $a_1 = 0$, we have the trivial solution $f \equiv 0$. Therefore a_1 must be -1. For generic odd initial data, a_3 is nonzero, giving the exponent $\beta = 3/2$, and the coefficients of

higher order terms are determined uniquely by a_3. Otherwise, β is decided from the next nonvanishing term in the series.

Actually, we can directly integrate (2.11) to get an implicit algebraic equation for f. Multiplying both sides of the differential equation (2.11) by $f(y)^{-(2\beta-1)/(\beta-1)}$ and taking the integration once, we get

$$(2.14) \qquad f(y)^{-\frac{1}{\beta-1}}\left(1+\frac{y}{f(y)}\right) = c_1$$

for some finite constant c_1. Since the above equation holds in the limit when $y \to 0$, $f(y)$ must be $-y + o(y)$ such that $1 + y/f(y)$ vanishes at the origin. Applying the condition that the limit exist once more, we find that the next higher order term of $f(y)$ must be of the form

$$(2.15) \qquad f(y) = -y + c_1(-y)^{\frac{\beta}{\beta-1}} + o\left((-y)^{\frac{\beta}{\beta-1}}\right).$$

Therefore, the exponent β is determined by the second nonvanishing term of the profile, which is ultimately determined by the initial condition. For generic even initial condition u_0, $f(y)$ is odd and the next nonvanishing term is cubic, giving $\beta/(\beta-1) = 3$, or $\beta = 3/2$. This *anomalous* exponent is consistent with the lower bound from numerical simulation in the next section.

However, this special trick and these special solutions do not seem to carry over to higher dimensions. Unlike the nonlinear filtration problem, the exponents cannot be derived using perturbation [2] or renormalization group methods [31] from known solutions in special cases or for some "unperturbed" problems. For this reason, high resolution numerical simulations are an important tool for uncovering the detailed dynamics of the blowup in higher dimensions. We summarize our results from such simulations in the next subsection.

2.2. Numerical observations of the blowup dynamics. Here we use the same U to denote the blowup profile at different times and its final steady state, and later even the radially symmetric profile, when no confusion could arise. Moreover, it is easy to check that if $U(y)$ is a solution of (2.7), so is

$$(2.16) \qquad U_\lambda(y) = \lambda^{n-1}U(\lambda y), \quad \lambda > 0,$$

and we have a family of profiles. Without loss of generality, any blowup profile shown below is normalized according to the above scaling such that $U(0) = 1$.

Details of the numerical methods are presented later in this manuscript. The overall results show exact self-similar scaling in all dimensions studied. The normalized profiles ($U(0) = 1$) obtained from our simulations of the PDE, in different spatial dimensions, are shown in Figure 1. Near the origin, the profiles are not ordered according to the dimension. But far away from the origin, due to different algebraic decay rates in different dimensions, these profiles are ordered. The algebraic tails (appearing as straight lines in the right log-log plot) will extend to infinity at the blowup time. The plot on the right shows a drop-off due to the matching of the numerical solution onto an integral order solution in the far field. Once we have the profiles, we can numerically check the validity of (2.7), which is shown in Figure 2 for dimension three. We observe that the part $\alpha U + \beta y \cdot \nabla U$ coming from the spatial-temporal scaling converges faster to a limit than the part associated with the kernel $\nabla \cdot (U \nabla K * U)$.
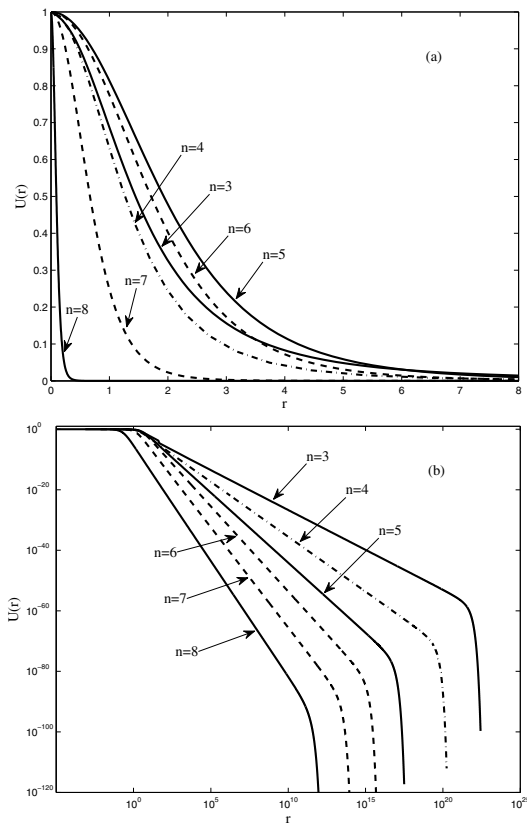
FIG. 1. *Similarity solution profiles show in the similarity variables U and $r = |y|$ as defined in (2.1)–(2.2), in different space dimensions, obtained by numerical integration of the PDE. All profiles are rescaled so that $U(0) = 1$ according to (2.16).*
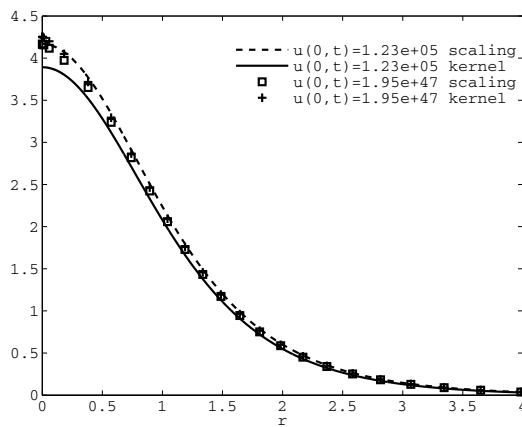

FIG. 2. *Comparison of the two contributions $\nabla \cdot (U \nabla K * U)$ (kernel) and $\alpha U + \beta y \cdot \nabla U$ (scaling) in (2.7) for different $u(0, t)$ in dimension three. The term $\alpha U + \beta y \cdot \nabla U$ (dashed line) at smaller values of $u(0, t)$ is almost indistinguishable from both terms at larger values of $u(0, t)$.*
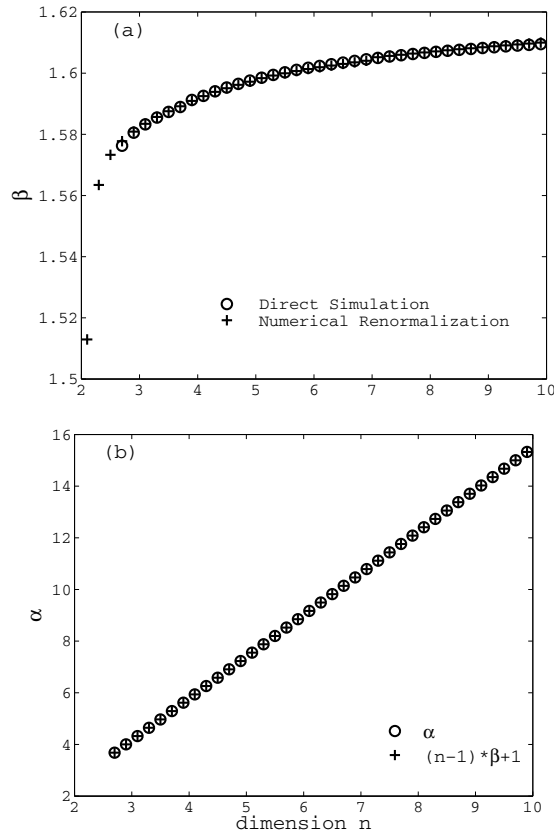
Fig. 3. *The exponents β and α characterizing the blowup in different spatial dimensions. In (a), because of the singularity of ∇K and ΔK, the exponent β can be computed accurately only for dimensions not less than three in the direct simulation. In (b) the relation (2.5) is verified numerically for direct simulation of the blowup dynamics.*

Both of the exponents α and β (Figure 3) are estimated by fitting the simulation data. For radially symmetric solutions considered here, the computation can be extended to fractional dimension, giving more insight into the dependence of the parameters on the spatial dimension. In particular, the parameter β appears to increase with dimension.

We can have a closer look at the detailed blowup scenario in Figures 4 and 5 for the rescaled profile U and the original function u. Even though the results are presented only in dimension three, it is generic for all dimensions. In Figure 4, the rescaled profiles $U(r, \tau)$ converge to the steady state quickly near the origin and the dynamics adjusts only the algebraic decay of the tails. In Figure 5, the original variable u is plotted at a different stage during the blowup. Since the blowup takes place in such a short time, away from the core u barely changes. Near the blowup point, the solution fills an envelope when approaching the blowup time. Moreover, the algebraic decay rates of u and U are intimately related through the self-similar relation (2.2). In fact any fixed $|x| > 0$, $u(x, t) = (T-t)^{-\alpha} U(x(T-t)^{-\beta}, \tau)$ approaches a constant as $t \to T^-$. This gives the rate of algebraic decay for the steady profile U, $U(y) \sim |y|^{-\alpha/\beta} = |y|^{-(n-1+1/\beta)}$, making the part $\alpha U + \beta y \cdot \nabla U$ in (2.7) vanish at leading order.
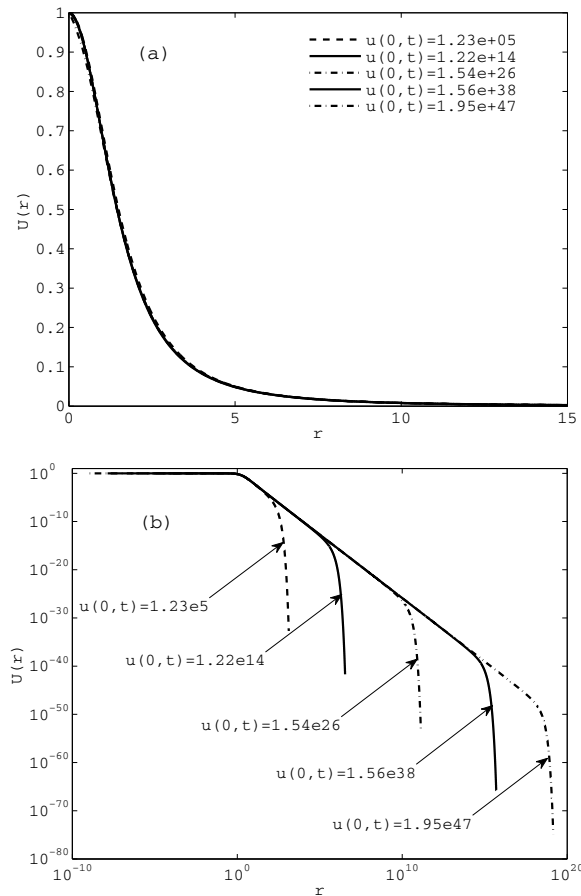
FIG. 4. *The convergence of the normalized profiles in dimension three.* (a) *Near the origin, all the profiles are indistinguishable.* (b) *Far away from the origin, the blowup dynamics adjusts the algebraic decay of the tail.*

3. Numerical methods. The computation of blowup solutions is usually quite challenging, due to the small scale of the blowup set, which cannot be resolved as well by conventional numerical schemes. One of the most popular schemes is the moving mesh method [18, 15, 34], using an equipartition principle to give a separate equation for the mesh, to concentrate the computation on those regions where high resolution is desired. Another one is dynamic rescaling used in nonlinear Schrödinger equations (see [42] and [27]). However, most of these schemes require a knowledge of those exponents characterizing the blowup to capture the dynamics accurately. Therefore they tend to work more successfully for self-similar solutions of the first kind.

Here we take advantage of the fact that our problem is a first order transport equation with a nonlocal velocity, and thus we can use the method of characteristics to solve two coupled ODEs, one for the radial position r and the other for the solution u. In radial coordinates, the original equation can be written as

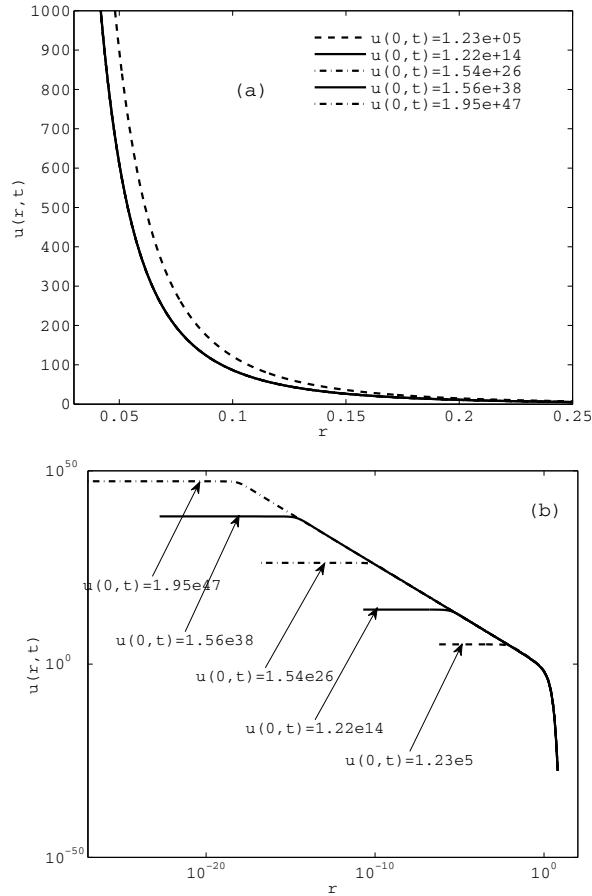$$(3.1) \qquad u_t = \frac{\partial u}{\partial r}\frac{\partial}{\partial r}K * u + u\Delta_r K * u,$$

FIG. 5. *The convergence of the original function u in dimension three.* (a) *Away from the blowup point, the solution barely changes because the blowup happens in such a short time scale.* (b) *Close to the blowup point, the solution fills an envelope which becomes infinity at the origin.*

where $\Delta_r = \partial_{rr} + \frac{n-1}{r}\partial_r$. The system of ODEs along the characteristics is thus

$$(3.2) \qquad \frac{dr}{dt} = -\frac{\partial}{\partial r}K * u, \quad \frac{du}{dt} = u\Delta_r K * u.$$

The method of characteristics is used in many of the analytical arguments to prove the existence and other important properties of the aggregation equation (1); see [12] and [6]. This method provides a natural adaptive grid scheme to concentrate spatial resolution near the blowup point or set, and was employed to investigate gravitational collapse by Brenner and Witelski [14]. Moreover, for nonnegative initial data, we have the monotonicity condition $\frac{\partial}{\partial r}K * u \geq 0, \Delta_r K * u > 0$; i.e., the points always move towards the origin and the magnitude is always increasing along the path. Thus our scheme preserves the positivity of the solution. The numerical results indicate that this simple scheme resolves the profiles quite well, both near the core and far away from it. If the self-similarity were of the first kind, then the characteristics would exactly preserve the spatial resolution going into the blowup. Since it is a second-kind similarity solution with anomalous scaling (i.e., the characteristics do not scale

in time as the similarity variable) we lose resolution over time, but at a relatively slow rate compared with the dynamics of blowup.

The system (3.2) is solved using the conventional fourth order Runge–Kutta method, with the size of the time step Δt adapted according to the following two criteria: (a) The relative increase of the solution at all points is bounded by a threshold at each time step. (b) The nodes cannot cross each other during each time step. Finally, we need to compute the convolution of the kernel. We first give a general formulation for any dimension greater than two and then a special one in odd dimensions three and higher to reduce computational effort by one order of magnitude.

3.1. General dimension. Instead of calculating $K * u$ once and taking the numerical derivatives to solve (3.2), we find $\frac{\partial}{\partial r} K * u$ and $\Delta_r K * u$ directly by computing the derivatives of the kernel, i.e.,

$$(3.3) \qquad \frac{\partial}{\partial r} K * u = c_n \int_0^\infty u(r') r'^{n-1} \int_0^\pi \frac{r - r' \cos\theta}{\sqrt{r^2 + r'^2 - 2rr' \cos\theta}} \sin^{n-2}\theta \, d\theta dr',$$

$$\Delta_r K * u = (n-1) c_n \int_0^\infty u(r') r'^{n-1} \int_0^\pi \frac{1}{\sqrt{r^2 + r'^2 - 2rr' \cos\theta}} \sin^{n-2}\theta \, d\theta dr',$$

where c_n is the volume of the unit sphere in R^{n-1}. The computation can still be expensive, because at each point we have to perform a double integration. The expense can be reduced by observing the homogeneity of the kernel, which gives the following formulation:

$$\int_0^\pi \frac{r - r' \cos\theta}{\sqrt{r^2 + r'^2 - 2rr' \cos\theta}} \sin^{n-2}\theta \, d\theta = \begin{cases} \int_0^\pi \frac{(1 - \rho\cos\theta)\sin^{n-2}\theta}{\sqrt{1 + \rho^2 - 2\rho\cos\theta}} d\theta & \text{if } r' \le r, \\ \int_0^\pi \frac{(\rho - \cos\theta)\sin^{n-2}\theta}{\sqrt{1 + \rho^2 - 2\rho\cos\theta}} d\theta & \text{if } r' \ge r, \end{cases}$$

$$(3.4) \qquad \int_0^\pi \frac{\sin^{n-2}\theta}{\sqrt{r^2 + r'^2 - 2rr'\cos\theta}} d\theta = \frac{1}{\max(r,r')} \int_0^\pi \frac{\sin^{n-2}\theta}{\sqrt{1 + \rho^2 - 2\rho\cos\theta}} d\theta,$$

where $\rho = \min(r,r')/\max(r,r')$. In this way, the integrations of the kernel with respect to the angular variable have to be calculated only once at the very beginning as functions of $\rho \in [0,1]$; i.e., we only need to perform numerical integrations once for the auxiliary functions

$$(3.5) \qquad I_1(\rho) = \int_0^\pi \frac{(1 - \rho\cos\theta)\sin^{n-2}\theta}{\sqrt{1 + \rho^2 - 2\rho\cos\theta}} d\theta, \quad I_2(\rho) = \int_0^\pi \frac{(\rho - \cos\theta)\sin^{n-2}\theta}{\sqrt{1 + \rho^2 - 2\rho\cos\theta}} d\theta,$$

$$(3.6) \qquad I_3(\rho) = \int_0^\pi \frac{\sin^{n-2}\theta}{\sqrt{1 + \rho^2 - 2\rho\cos\theta}} d\theta.$$

The auxiliary variable ρ is chosen such that those integrations are computed only at discrete points and the interpolations of $I_1, I_2,$ and I_3 are restricted on the bounded interval $[0, 1]$. Therefore functions $I_1, I_2,$ and I_3 can be computed as accurately as needed without increasing the computational effort during the time evolution. In this way the total computational expense is reduced to $O(N^2)$ at each time step, where N is the number of spatial points used to represent the solution. These auxiliary functions (Figure 6) are relatively smooth inside the interval $[0, 1]$ for dimension greater than or equal to three. It is easy to see that $I_3(1)$ actually becomes divergent for dimensions n less than or equal to two. For these reasons, the computations are performed only for $n > 2$.
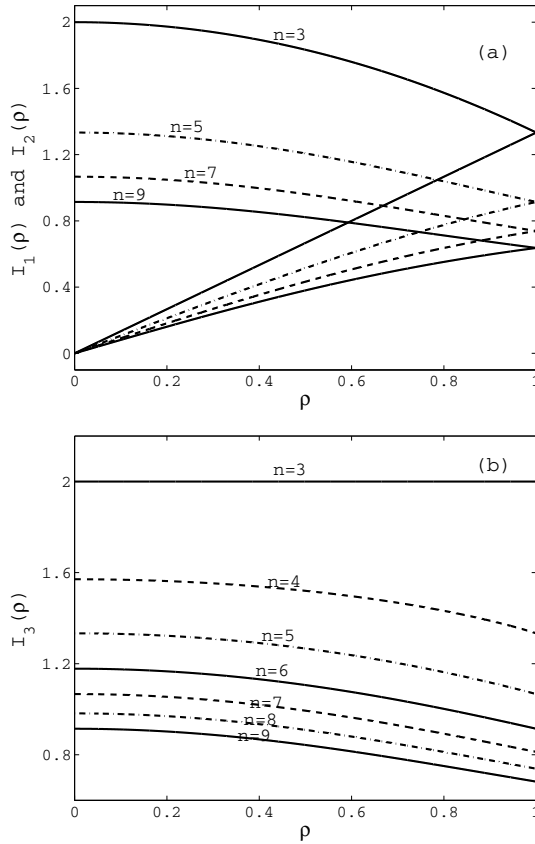
FIG. 6. *Auxiliary functions in different spatial dimensions:* (a) I_1 *(upper branch) and* I_2 *(lower branch),* (b) I_3.

3.2. Further reduction in odd dimensions. In odd dimensions, using the fact that the successive Laplacians of the kernel $K(x) = |x|$ is proportional to the fundamental solution of the Laplace equation, we can further reduce the computation to $O(N)$ per time step. This is exactly the fact used to prove the nonexistence of mass-concentrating self-similar solutions in [7]. First, we start with dimension three to give the basic idea and then generalize it to any odd dimension greater than three. Let $v_0 = u$, and define v_1 and v_2 to be the solutions of the equations

$$(3.7) \qquad\qquad -\Delta v_1 = v_0, \quad \Delta v_2 = 8\pi v_1 \quad \text{in } R^3,$$

with v_1 and v_2 decaying to zero at infinity. Using the explicit formula for the solution of the Poisson equation, we obtain

$$v_1(x) = \int_{R^3} \frac{v_0(y)}{4\pi|x-y|} dy,$$

$$v_2(x) = \int_{R^3} \frac{2v_1(y)}{|x-y|} dy = \int_{R^3}\int_{R^3} \frac{v_0(z)}{2\pi|x-y||y-z|} dz\,dy$$

$$(3.8) \qquad\qquad = \int_{R^3} |x-z|v_0(z)dz = K * v_0(x).$$

In the radial symmetric case, we only need to solve

$$(3.9) \qquad -\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dv_1}{dr}\right) = v_0, \quad -\frac{1}{r^2}\frac{d}{dr}(r^2 v_{2r}) = 8\pi v_1,$$

with the boundary condition

$$(3.10) \qquad v_1(\infty) = 0, \quad \frac{\partial v_1(0)}{\partial r} = 0, \quad v_{2r}(0) = 0.$$

Then the right-hand sides of the equations in (3.2) are replaced by

$$(3.11) \qquad \frac{\partial}{\partial r}K * u = -v_{2r}, \quad \Delta_r K * u = 8\pi v_1,$$

with the time scaled by 8π. Note that we only need to find the derivative $\partial_r v_2$ of v_2, instead of v_2 itself. In actual implementation, the infinity boundary condition $v_1(\infty) = 0$ is transformed into a condition at $r = 0$, i.e., the value of $v_1(0)$,

$$(3.12) \qquad v_1(0) = -\int_0^\infty \frac{\partial v_1(r)}{\partial r}dr = \int_0^\infty \frac{1}{r^2}\int_0^r v_0(s)s^2 ds dr = \int_0^\infty u(r)r dr.$$

This integral is usually truncated on a bounded domain if u is compactly supported or decays fast enough. In theory, this transformed boundary condition at the origin gives the unique zero boundary condition at infinity, while any inappropriate choice of v_1 at the end of the computational domain (an approximation to the condition $v_1(\infty) = 0$) could give a different effective kernel K, resulting in some inconsistency in theory and numerics. Once we have the right boundary condition, we can use an $O(N)$ numerical quadrature scheme to find the solution of (3.9), i.e.,

$$v_1(r) = v_1(0) - \int_0^r \frac{1}{\eta^2}\int_0^\eta u(s)s^2 ds d\tau = v_1(0) - \int_0^r u(s)\left(s - \frac{s^2}{r}\right)ds,$$

$$(3.13) \quad v_{2r}(r) = \frac{8\pi}{r^2}\int_0^r v_1(s)s^2 ds.$$

In odd dimensions greater than three, with $n = 2k + 1$, similarly we introduce $v_1, v_2, \ldots, v_{k+1}$ such that

$$(3.14) \qquad -\Delta v_1 = v_0, \ -\Delta v_2 = v_1, \ \ldots, \ -\Delta v_k = v_{k-1}, \ \Delta v_{k+1} = d_k v_k \quad \text{in } R^n$$

and finally set in the characteristic ODEs (3.2)

$$(3.15) \qquad \frac{\partial}{\partial r}K * u = -\frac{\partial v_{k+1}}{\partial r}, \quad \Delta_r K * u = d_k v_k,$$

where $v_0 = u$ and

$$(3.16) \qquad d_k = 2^k(2k+1)k!\frac{\pi^{\frac{2k+1}{2}}}{\Gamma(k+1+\frac{1}{2})}.$$

To transform the boundary condition at infinity into the one at the origin, we need to find an appropriate integration such as (3.12) with the aid of a fundamental solution of the Laplace equation, which is given by

$$(3.17) \qquad N(x) = \frac{1}{n(n-2)\omega_n|x|^{n-2}}, \quad \omega_n = \frac{\pi^{n/2}}{\Gamma(n/2+1)},$$

where ω_n is the volume of the unit sphere in R^n. Using the presentation formula of the solution to the Poisson equation, we have

(3.18)
$$v_i(x_i) = \int_{R^n} \cdots \int_{R^n} N(x_i - x_{i-1})N(x_{i-1} - x_{i-2}) \cdots N(x_1 - x_0)u(x_0)dx_0 dx_1 \cdots dx_{i-1}$$

for any $1 \le i \le k+1$. Translation and rotation invariance of the fundamental solutions give the identity

(3.19)
$$\int_{R^n} \cdots \int_{R^n} N(x_i - x_{i-1})N(x_{i-1} - x_{i-2}) \cdots N(x_1 - x_0)dx_1 \cdots dx_{i-1} = N_i(x_i - x_0)$$

for some radially symmetric function N_i. Moreover, dimensional analysis indicates that N_i is homogeneous of degree $2i - n$, i.e.,

(3.20)
$$N_i(x_i - x_0) = \frac{c_{i,n}}{n\omega_n}|x_i - x_0|^{2i-n}$$

for some constant $c_{i,n}$. When $i = 1$, this is just the fundamental solution, giving the following initial condition:

(3.21)
$$c_{1,n} = \frac{1}{n-2}.$$

We can find a recursive relation for $c_{i,n}$ by taking the negative Laplacian of N_i with respect to x_i. Formally, on one hand using (3.20),

(3.22)
$$-\Delta_{x_i} N_i(x_i - x_0) = \frac{2(n - 2i)(i - 1)c_{i,n}}{n\omega_n}|x_i - x_0|^{2(i-1)-N}.$$

On the other hand, using the definition of N_i,

$$-\Delta_{x_i} \int_{R^n} \cdots \int_{R^n} N(x_i - x_{i-1})N(x_{i-1} - x_{i-2}) \cdots N(x_1 - x_0)dx_1 \cdots dx_{i-1}$$

$$= \int_{R^n} \cdots \int_{R^n} \delta(x_i - x_{i-1})N(x_{i-1} - x_{i-2}) \cdots N(x_1 - x_0)dx_1 \cdots dx_{i-1}$$

$$= \int_{R^n} \cdots \int_{R^n} N(x_i - x_{i-2}) \cdots N(x_1 - x_0)dx_1 \cdots dx_{i-2}$$

(3.23)
$$= \frac{c_{i-1,n}}{n\omega_n}|x_i - x_0|^{2(i-1)-N}.$$

Matching the coefficients of the above two identities, we have the recursive formula

(3.24)
$$c_{i,n} = \frac{1}{2(i - 1)(n - 2i)}c_{i-1,n},$$

and consequently with the initial condition (3.21),

(3.25)
$$c_{i,n} = \frac{1}{2^{i-1}(i - 1)!(n - 2i)!!},$$

where $m!!$ is the double factorial of m. Finally, we get the boundary condition of v_i at the origin in terms of the integral with u, i.e.,

(3.26) $$v_i(0) = \frac{c_{i,n}}{n\omega_n} \int_{R^n} |x_0|^{2i-n}u(x_0)dx_0 = \frac{1}{2^{i-1}(i - 1)!(n - 2i)!!} \int_0^\infty r^{2i-1}u(r)dr.$$

With these boundary conditions, we can find all the auxiliary functions v_i's through a series of $O(N)$ numerical integrations like (3.13) to find the right-hand side of the characteristic ODEs (3.2).

3.3. Numerical renormalization group. Since we are more interested in the exponents characterizing the intermediate asymptotics of the dynamics than other quantitative details, we can rescale the solution appropriately to get the profile. This is the basic principle underlying the renormalization group method, which is employed successfully to the numerical investigation of nonlinear filtration and porous medium equations [23, 11].

We start with the solution $u^{(0)}(x,t) = u(x,t)$, which is known on the time interval $[t_0^0, t_1^0]$. Without loss of generality, we let $u^{(0)}(0, t_0^0) = 1$, and t_1^0 is determined implicitly by $u^{(0)}(0, t_1^0) = M$ for some predetermined constant $M > 1$. For a given guess of the exponent β_m, at the end of the mth iteration, we can renormalize the function as

$$(3.27) \qquad u^{(m+1)}(x, t_0^{m+1}) = M^{-1} u^{(m)}(x M^{-\beta_m/\alpha_m}, t_1^m), \qquad \alpha_m = (n-1)\beta_m + 1.$$

An equation for β_m can be estimated from the spatial-temporal relation of the blowup dynamics. Near blowup time, we have

$$(3.28) \qquad u(0,t) = (T-t)^{-\alpha} U_0, \qquad r_{1/2}(t) = (T-t)^\beta r_0,$$

where $r_{1/2}(t)$ is the position in which u is half of u at the origin, i.e.,

$$(3.29) \qquad u(r_{1/2}(t), t) = \frac{1}{2} u(0, t).$$

Therefore, on one hand we have

$$(3.30) \qquad \frac{d \ln u(0,t)}{d \ln r_{1/2}(t)} = \frac{d \ln u(0,t)/dt}{d \ln r_{1/2}(t)/dt} = -\frac{\alpha}{\beta} = 1 - n - \frac{1}{\beta}.$$

On the other hand, using the original evolution equation, we can calculate the time derivatives explicitly, i.e.,

$$(3.31) \qquad \frac{d \ln u(0,t)}{d \ln r_{1/2}(t)} = \frac{r_{1/2}(t)}{u(0,t)} \frac{du(0,t)/dt}{dr_{1/2}(t)/dt} = \frac{r_{1/2}(t)}{u(0,t)} \frac{\nabla \cdot (u \nabla K * u)|_{r=0}}{dr_{1/2}(t)/dt}.$$

Finally $dr_{1/2}(t)/dt$ can be obtained by taking the time derivative of (3.29),

$$(3.32) \qquad u_r(r_{1/2}(t), t) \frac{dr_{1/2}(t)}{dt} + u_t(r_{1/2}(t), t) = \frac{1}{2} u_t(0, t),$$

or equivalently

$$(3.33) \qquad \frac{dr_{1/2}(t)}{dt} = \frac{\frac{1}{2} \nabla \cdot (u \nabla K * u)|_{r=0} - \nabla \cdot (u \nabla K * u)|_{r=r_{1/2}(t)}}{u_r(r_{1/2}(t), t)}.$$

At the end of the mth iteration, the exponent β_m is solved by combining (3.30) and (3.31), i.e.,

$$(3.34)$$
$$1 - n - \frac{1}{\beta_m} = \frac{r_{1/2}(t_1^m)}{u^{(m)}(0, t_1^m)} \frac{u_r^{(m)}(r_{1/2}(t_1^m), t_1^m) \nabla \cdot (u^{(m)} \nabla K * u^{(m)})|_{r=0}}{\frac{1}{2} \nabla \cdot (u^{(m)} \nabla K * u^{(m)})|_{r=0} - \nabla \cdot (u^{(m)} \nabla K * u^{(m)})|_{r=r_{1/2}(t_1^m)}}.$$

The above relation is preserved under the renormalization transformation (3.27), in the sense that

$$(3.35) \quad 1 - n - \frac{1}{\beta_m}$$
$$= \frac{r_{1/2}(t_0^{m+1})}{u^{(m+1)}(0, t_0^m)} \frac{u_r^{(m+1)}(r_{1/2}(t_0^{m+1}), t_0^{m+1}) \nabla \cdot (u^{(m+1)} \nabla K * u^{(m+1)})|_{r=0}}{\frac{1}{2} \nabla \cdot (u^{(m+1)} \nabla K * u^{(m+1)})|_{r=0} - \nabla \cdot (u^{(m+1)} \nabla K * u^{(m+1)})|_{r=r_{1/2}(t_0^{m+1})}}.$$

Because the renormalized function decays only algebraically even with a compactly supported initial data, the function $u^{(m)}$ is computed on an interval $r \in [0, L]$ and is chosen to be $u(L)(L/r)^{\alpha_m/\beta_m}$ for $r > L$.

The anomalous exponent β computed using this numerical renormalization method is compared with that from direct simulation in Figure 3. The former concentrates the computation on the profile and the exponents with a fixed spatial domain, while the latter has to resolve the solution on a large spatial domain and eventually cannot give a good fit at lower dimensions when the kernel becomes singular. Therefore, the profile and the exponents can be computed with high accuracy without any formation of singularity. On the other hand, the direct simulation tells more details about the blowup dynamics, like various norms of the solution when approaching the blowup time.

For simulation in general dimensions, the auxiliary functions I_1, I_2, and I_3 are computed on 10^4 equally spaced points on the interval $[0, 1]$. The number of spatial points is 4000 and the whole simulation takes a few days for one single dimension on a 3.0 GHz Intel Pentium IV cluster machine compiled with GNU GCC. For the special formulation in odd dimensions, the number of spatial points is as large as 2×10^4, and the simulation usually takes a few hours. Initially the grid points $\{r_j\}$ are placed such that $\ln(1 + r_j)$ is equally spaced on $[0, \ln(1 + r_N)]$. The initial condition is chosen to be Gaussian, even though other smooth, compactly supported functions (not necessarily radially decreasing) work well too and produce computationally identical similarity solutions. The special code for simulation in odd dimensions gives exponents α and β and other parameters consistent with code for general dimensions. The main difference is computational speed. We reiterate that we do not have to perform adaptive mesh refinement because the characteristics do a good job of following the similarity variables, although they are not identical.

4. Additional numerical results. Besides those results already shown in previous sections, we gather addition numerical results and verifications to validate the claims made before.

4.1. Estimation of the exponents. Close to the blowup time, $U(0, \tau)$ should approach a constant U_0, and $u(0, t) \sim (T - t)^{-\alpha} U_0$. The time derivative $u_t(0, t)$ can be approximated by $u(0, t)$ too, i.e.,

$$(4.1) \qquad u_t(0, t) \sim \alpha U_0^{-1/\alpha} u(0, t)^{1+1/\alpha}.$$

On the other hand, from the second characteristic ODE (3.2), $u_t(0, t) = u(0, t)\Delta_r K * u(0, t)$, we have

$$(4.2) \qquad \ln\left(\Delta_r K * u(0, t)\right) = \ln(\alpha U_0^{-1/\alpha}) + \frac{1}{\alpha} \ln u(0, t).$$

Using $u(0, t), \Delta_r K * u(0, t)$ at each time step, a simple least squares fitting gives the pair of parameters (α, U_0), as in Figure 7(a). To estimate the exponent β for spatial spread, we need to introduce a spatial scale. The most natural one is the half-width of the blowup profile, $r_{1/2}(t)$, the position at which the magnitude is half of that at the origin, i.e.,

$$(4.3) \qquad u(r_{1/2}(t), t) = u(0, t)/2.$$

The similarity form of the blowup implies

$$(4.4) \qquad r_{1/2}(t) \sim r_0(T - t)^\beta \sim r_0 U_0^{\beta/\alpha} u(0, t)^{-\beta/\alpha}$$
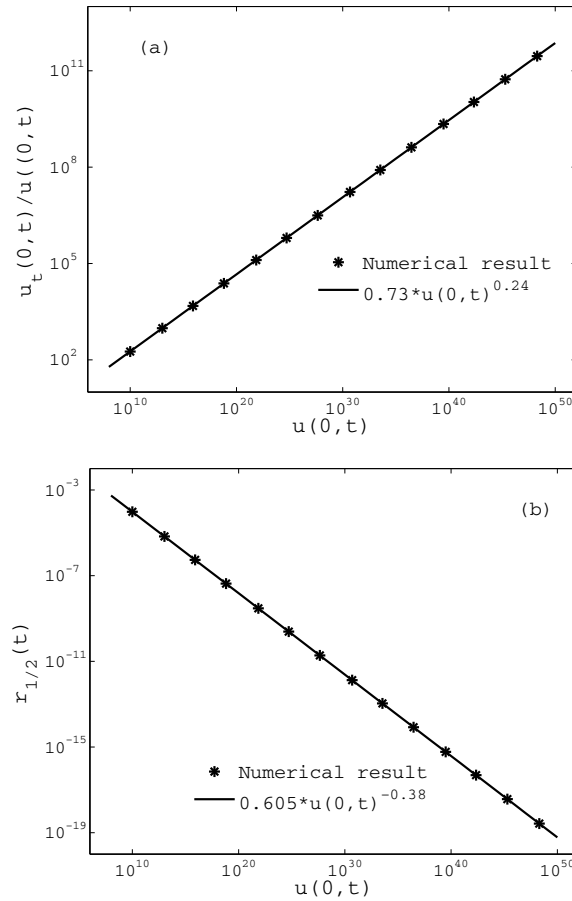
FIG. 7. *Estimation of $\alpha\,(\approx 1/0.24 = 4.167)$ and $\beta\,(\approx 0.38/0.24 = 1.583)$ in dimension three by fitting.*

for some constant r_0. Using $r_{1/2}(t)$ (from interpolation if there is no function value that is exactly half of the maximum magnitude) and $T-t$ estimated with parameters obtained above, we can get β, as in Figure 7(b). In all the parameter estimations, only those data close to blowup time $(u(0,t) > 10^{10})$ are used, and the profiles should be radially decreasing such that there is one unique $r_{1/2}(t)$. The simulation is terminated when $u(0,t)$ reaches an upper bound 10^{50}, provided that the profile near the origin is well resolved—say, for example, there are at least one hundred node points on the interval $[0, r_{1/2}(t)]$.

4.2. Blowup in the L^p norm. Since the blowup does not concentrate any mass, it is possible that the L^p norm of the solution could still be finite for some $p > 1$ at the blowup time. Using the self-similar form verified in previous sections, we can give a more quantitative characterization of the blowup in the L^p norm. First, we have

(4.5)
$$||u||_{L^p}^p = \int_{R^n} u^p dx = (T-t)^{-\alpha p + n\beta} \int_{R^n} U^p dy = (T-t)^{-\alpha p + n\beta} C \int_0^\infty U^p r^{n-1} dr.$$

Let the critical exponent be defined as $p^* = n\beta/\alpha$. To the leading order, U has an algebraic decay rate of the form $r^{-\alpha/\beta}$, and this rate of decay is extended to infinity as $t \to T$. If $p > p^*$, the integrand $U^p r^{n-1}$ decays fast enough and the last integral in (4.5) is uniformly bounded and nonzero; therefore the behavior of $||u||_{L^p}$ is determined by $(T - t)^{-\alpha(1-p^*/p)}$, which becomes infinity.

For $p \in (1, p^*)$, the integral in the last expression blows up but the factor $(T - t)^{-\alpha p + n\beta}$ goes to zero. Therefore, we need a more delicate estimate for the integral using the fact that U has an algebraic decay only up to some large distance $R(t)$. This upper bound can be estimated from the total mass for U. On one hand, from the evolution equation for U, we have

$$(4.6) \qquad \frac{d}{d\tau} \int_{R^n} U(y, \tau) dy = (\beta - 1) \int_{R^n} U(y, \tau) dy$$

or

$$(4.7) \quad \int_{R^n} U(y, \tau) dy = e^{(\beta-1)\tau} \left[e^{(\beta-1)\ln T} \int_{R^n} U(y, -\ln T) dy \right] = (T - t)^{-(\beta-1)} M_0,$$

where M_0 is a constant depending only on the initial condition. On the other hand, the integral above can be approximated by assuming $U(y, \tau)$ has an algebraic decay of order $O(|y|^{-\alpha/\beta})$ exactly up to $R(t)$ and is zero beyond $R(t)$, i.e., for t close to the blowup time T,

$$\int_{R^n} U(y, \tau) dy \approx \int_{R_0}^{R(t)} C r^{-\alpha/\beta + n - 1} dr \approx C_1 R(t)^{n - \alpha/\beta} = C_1 R(t)^{1 - 1/\beta}.$$

Compared with (4.7),

$$R(t) \approx C_2 (T - t)^{-\beta}$$

and consequently the L^p norm is
(4.8)
$$||u||_{L^p}^p \approx C (T - t)^{-\alpha p + n\beta} \int_0^{R(t)} r^{-\alpha p/\beta + n - 1} dr = C_1 (T - t)^{-\alpha p + n\beta - \beta(-\alpha p/\beta + n)} = C_1.$$

In other words, if $p \in (1, p^*)$, $||u||_{L^p}$ is still uniformly bounded up to blowup time.

At the critical norm $p = p^*$,

$$(4.9) \qquad ||u||_{L^{p^*}}^{p^*} \approx C \int_{R_0}^{R(t)} r^{-1} dr = C_1 + C_2 \ln R(t) = C_1 - C_2 \beta \ln(T - t).$$

For all three cases, the above analysis is in perfect agreement with numerical observation of the norms (Figures 8 and 9). The total mass $||u||_{L^1}$ is still perfectly conserved even for $u(0, t)$ close to 10^{50}. In the critical ($p = p^*$) and supercritical ($p > p^*$) cases, the blowup of the norms fits the expected form of logarithm and power law blowup very well. This blowup result is also consistent with the L^p theory developed in a companion paper [10], in which the local well-posedness of the equation is proved for initial data in L^p space with p greater than $p_s = n/(n-1) > p^*$. At the time of blowup, our numerical solution exhibits a pure power law behavior at the origin. In [10] it is shown that continuation of a solution of this type leads to instantaneous mass concentration, hence proving that the dynamics is ill-posed in the L^p for sufficiently
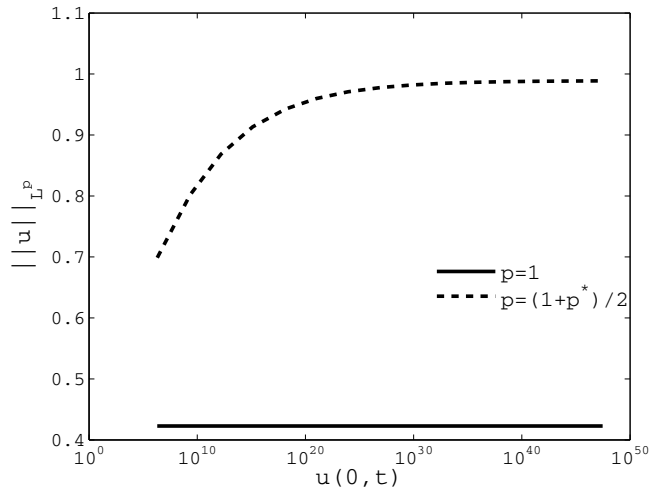
FIG. 8. $||u||_{L^p}$ for $p = 1$ and $p = (1 + p^*)/2$ $(< p^*)$ in dimension $n = 3$. Note that the mass $(p = 1)$ is perfectly conserved in our numerical scheme.
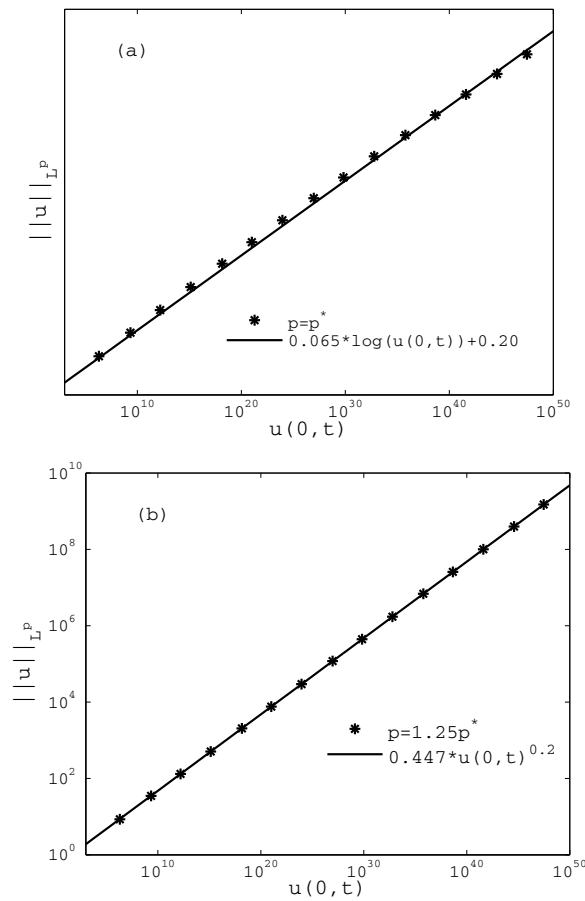

FIG. 9. Logarithmic blowup of $||u||_{L^p}$ for $p = p^*$ (a) and power law blowup for $p > p^*$ (b) in dimension $n = 3$. In the latter case $1/5$ is exactly the theoretic predicted value $1 - p^*/p$.

small p. Thus the numerical results here, combined with the analysis of that paper, give a complete picture of the dynamics, from smooth initial data to finite time blowup with a power law singularity, and then instantaneous mass concentration after the initial singularity. We note that this is a multidimensional generalization of how singularities form in the Burgers equation, which we have shown is equivalent to our problem in one dimension. In the Burgers case, the initial singularity for (2.10) involves $\phi(x, T) \sim x^{1/3}$ at the blowup time, which, following the classical theory of conservation laws, instantaneously leads to shock formation with a jump discontinuity, corresponding to mass concentration in the corresponding aggregation problem. Thus we see the same phenomena occurring in multiple dimensions.

5. Conclusions. We have studied the blowup behavior of solutions of the aggregation equation $u_t = \nabla \cdot (u \nabla K * u)$ in multiple dimensions for the kernel $K(x) = |x|$. The numerical observations give strong evidence that the solutions are self-similar and of the second kind. Even though the numerical results are consistent with known theory, in particular the lack of first-kind similarity solutions in odd dimensions higher than one [7], there are still many important questions left unanswered. First, the solutions are computed only in the radially symmetric case. However, this radial symmetry could be broken by a nonradially symmetric perturbation. We have not performed linear stability theory for this problem, as has been done in other examples of self-similarity [5], and this would be interesting, both for the radially symmetric and nonradial cases.

Likewise, we have not done a systematic study of solutions of the similarity equation (2.7)—as has been shown for other problems [26, 50], there may exist unstable similarity solutions with different shape from the ones found in this paper. Moreover, the homogeneity of the kernel can be generalized to $K(x) = |x|^{\gamma}$, which has been proposed for some one-dimensional models of granular flow [21, 41], and the dynamics of blowup for such kernels is an interesting open problem in multiple dimensions. We also note that there are recent theoretical results on blowup for this class of problems with additional linear and nonlinear diffusion [39, 40], and it would be interesting to understand blowup profiles for these problems as well. Our method of characteristics does not directly apply to such problems due to the diffusive nature of the dynamics. One possibility, which we have not discussed here, is to use ideas from optimal transport theory, which applies to this class of equations [7]. A recent numerical scheme built on this idea, for diffusive and aggregation phenomena, has been introduced in [22].

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