Geometric order parameter equations

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Abstract

Aggregation of particles whose interaction potential depends on their mutual orientation is considered. The aggregation dynamics is derived using a version of Darcy’s law and a variational principle depending on the geometric nature of the physical quantities. The evolution equations that result separate into two classes: either characteristic equations, or gradient flow equations. We derive analytical solutions of both types of equations which are collapsed (clumped) states and show their dynamical emergence from smooth initial conditions in numerical simulations.

Keywords: gradient flows, blow-up, chemotaxis, parabolic-elliptic system, singular solutions

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**Introduction** Many physical processes can be understood as aggregation of individual ‘components’ at a variety of scales into a final ‘product’. Diverse examples of such processes include the formation of stars, galaxies and solar systems at large scales, organization of insects and organisms into colonies at mesoscales and self-assembly of proteins, nanotubes or micro/nanodevices at micro- and nanoscales. Some of these processes, such as nanoscale self-assembly of molecules are of great technological interest. Of special interest is the case when the energy of interaction among the assembling particles depends not just on the distance, but also on mutual orientation. In particular, this Letter is motivated by recent experiments and simulations on self-assembly of non-circular particles (squares, hexagons etc.) Due to the large number of particles involved in self-assembly ($10^9 - 10^{12}$), the development of continuum descriptions for aggregation or self-assembly is a natural approach toward theoretical understanding and modeling.

Self-assembly at microscopic scales may be simpler than fluid dynamics, because the Reynolds number is so low that inertia is negligible. The classic examples of continuous equations for aggregation are those of Debye-Hückel and Keller-Segel (KS). For a recent review of developments in this area with an emphasis on biophysical modeling, see, for example. The physics of these models consists of a conservation law: $\partial_t \rho + \text{div}\rho u = 0$, coupled with an evolution equation for velocity $u$ which depends on the density $\rho$ through a free energy $E$ as $u \simeq \mu \nabla \delta E/\delta \rho$ (velocity proportional to force), in which ‘mobility’ $\mu$ may also depend on the density. This relation is known as “Darcy’s Law.” In most recent works (and references within) the energy $E$ is computed under the assumption that the interaction between the particles is central, i.e., that it does not depend on their orientation. This framework is simple and attractive. However, the self-assembly of some physical systems may depend on geometric properties such as the mutual orientation of pieces. Examples of such systems range from micro-biological (mutual attraction of cells, viruses or proteins), to electromagnetic (dipoles in continuous media, orientation of domains), to interactions of living organisms (swarms, herds, flocks, etc.)

The goal of this Letter is to formulate a procedure to derive and analyze evolution equations for systems that self assemble under a flow in which generalized ‘velocity’ is proportional to generalized ‘force.’ Although we aim to derive equations for orientation-dependent motion, we will also show that the procedure for obtaining such evolution equations applies generally for any type of continuum physical quantity. Thus, we obtain a family of evolution equations.
for physical quantities such as active scalars, momenta and fluxes. (A complete list of equations derived by our method is given in [10].) After these equations have been formulated, we discuss their most remarkable feature. Namely, they possess emergent solutions – or coherent structures – in which the self-assembly is *singular* (localized into delta functions). In addition, these localized singular solutions dominate the long-term dynamics. From the physical point of view, such localized, or quenched solutions would form the core of the processes of self-assembly and are therefore of great practical interest. Moreover, the formation of these localized solutions is driven by a combination of nonlinearity and nonlocality in an evolutionary process that admits an *analytical* description of their long-term dynamics.

**Geometric evolution equations** The general principle for deriving an evolution equation for the self-assembly of any continuum physical quantity \( \kappa \) may be stated as, “The local value of \( \kappa \) remains invariant along the characteristic curves of a flow, whose velocity depends on \( \kappa \) through an appropriate Darcy Law.” This principle may be formulated in symbols as, 
\[
d\kappa(x(t), t)/dt = 0 \quad \text{along} \quad dx/dt = u[\kappa].
\]
In the case of particle density \( \rho \) in \( n \)-dimensional space, for example, the number of particles \( \kappa = \rho \, d^n x \) has physical meaning. Hence, the time derivative of \( \kappa \) in this case invokes the fundamental chain rule for the product of the density function times the volume element, \( \kappa = \rho(x(t), t) \, d^n x(t) \). Preservation of this product along 
\[
dx/dt = u[\rho]
\]

in which the dependence of the velocity vector \( u[\rho] \) as a functional of \( \rho \) is yet to be determined. As mentioned above, the Darcy Law approach assumes that velocity \( u \) depends on density \( \rho \) through the gradient of the variation of free energy \( E \) (velocity proportional to ‘force’ with mobility \( \mu \)). This assumption leads to the expected continuity equation for density,
\[
\partial_t \rho = -\text{div}(\rho \nabla \delta E/\delta \rho)^\sharp,
\]
where sharp \( (\cdot)^\sharp \) denotes raising the vector index from covariant to contravariant, so its divergence may be taken. This gradient-flow method generalizes for other physical quantities with different geometrical meaning, by noticing that the invariance property \( d\kappa(x(t), t)/dt = 0 \) along \( dx/dt = u[\kappa] \) may be expressed mathematically as \( \partial \kappa/\partial t + L_{u[\kappa]} \kappa = 0 \), where \( L_{u[\kappa]} \) is the Lie derivative with respect to the vector field \( u = u \cdot \nabla \) of any geometrical quantity \( \kappa \) [14]. The key question for the physical modeling is to identify the analog of Darcy’s Law.
Namely, what is the vector field \( u[\kappa] \) when \( \kappa \) is an arbitrary geometrical quantity? A surprising clue leading to the geometrical analog of Darcy’s Law emerges when considering the spontaneous appearance of singularities in solutions of \( (2) \) for which \( \mu \) and \( \delta E/\delta \rho \) depend on the average density, rather than its pointwise value \([11, 12]\). Those singular solutions obey a weak form of the continuity equation \( (2) \), expressed by pairing it with an arbitrary smooth test function \( \phi \) and integrating twice by parts, as

\[
\langle \partial_t \rho, \phi \rangle = \langle \delta \rho, \delta E/\delta \rho \rangle \quad \text{to find}
\]

\[
\delta \rho = - \text{div} \rho \mu \nabla \phi = - \mathcal{L}_{u(\phi)} \rho \quad \text{so} \quad u(\phi) = (\mu \nabla \phi)^\sharp
\]

where spatial integration defines the real-valued pairing \( \langle \cdot, \cdot \rangle \) between densities and their dual space of scalar functions. This expression for the weak solutions of the continuity equation \( (2) \) provides the clue we seek for expressing Darcy’s Law for the self-assembly of an arbitrary geometric quantity \( \kappa \), not just a density.

The clue we seek emerges upon re-doing the previous integrations by parts slowly and carefully as

\[
\langle \partial_t \rho, \phi \rangle = - \langle \mathcal{L}_{u(\phi)} \rho, \delta E/\delta \rho \rangle = - \langle u(\phi), \rho \circ \delta E/\delta \rho \rangle = - \langle (\mu \circ \phi)^\sharp, \rho \circ \delta E/\delta \rho \rangle.
\]

Here, we have introduced the diamond \( (\circ) \) as the dual of the Lie derivative under integration by parts for any dual pair \( (\kappa, b) \) and any vector field \( u \), \( \langle \kappa \circ b, u \rangle = \langle \kappa, -\mathcal{L}_u b \rangle \). This suggests \( u(\phi) = (\mu \nabla \phi)^\sharp = - (\mu \circ \phi)^\sharp \). Using the definition of diamond again gives

\[
\langle \partial_t \rho, \phi \rangle = - \langle (\mu \circ \phi)^\sharp, \rho \circ \delta E/\delta \rho \rangle = - \langle \mathcal{L}_{(\mu \circ \phi)^\sharp} \mu, \phi \rangle
\]

Replacing \( \rho \rightarrow \kappa \) here generalizes \( (2) \) to any quantity \( \kappa \) in an arbitrary vector space. We shall derive the particular versions of this equation for several physical quantities \( \kappa \). The result is a set of novel nonlocal characteristic equations which possess localized solutions.

**Singular solutions for the Geometric order parameter (GOP) equation \( (4) \).** Numerical simulations show the development of singular solutions in \( \kappa \) for some types of \( \kappa \) (e.g., scalars) and the absence of those singularities for other \( \kappa \)’s (e.g., vector fields). These solutions are reminiscent of the clumpon singularities \([11, 12]\), which dominate the long term...
dynamics once they have formed. Thus, we seek a particular solution of (4) expressed as a \( \delta \)-function parametrized by coordinate(s) \( s \) on a submanifold of ambient space,

\[
\kappa(x, t) = \int p(s, t) \delta (x - q(s, t)) \, ds .
\]

(5)

To derive the equations for \( p(s, t) \) and \( q(s, t) \), we substitute (5) into (4) and integrate the right-hand side by parts to extract the term proportional to \( \kappa \) as follows:

\[
\frac{\partial p}{\partial t} \phi (q(s, t)) + \frac{\partial q}{\partial t} \cdot \nabla \phi (q(s, t)) = \langle \kappa, \mathcal{N}_\kappa \phi \rangle
\]

(6)

where \( \mathcal{N}_\kappa \) is a linear operator acting on \( \phi \) depending on the nature of \( \kappa \). For example, for densities \( \kappa = \rho d^3 x \), \( \mathcal{N}_\kappa \phi = -\mu \nabla \delta E/\delta \rho \cdot \nabla \phi (q(s, t)) \). If the right-hand side of (6) only contains the function \( \phi \) and its gradient, then singular solutions (5) are possible. However, one must be careful because this condition could be over-determined and thus the existence of singular solutions of (4) for the evolution of an arbitrary geometric quantity might not be guaranteed. Two classes of geometric quantities admitting singular solutions of (4) are known [10]. One class includes, for example, scalars, 1-forms and 2-forms, and gives characteristic equations for which the characteristic velocity is a nonlocal vector function. A second class, which encompasses in particular an orientation-dependent density, is a nonlinear nonlocal diffusion equation. In each case, one must compute the particular expression for the right hand side of (4), and integrate by parts to extract the function \( \phi \) and its derivatives.

Since our main interest lies with the second case, we shall describe the nonlocal characteristic equations only very briefly. It is essential to discuss them, however, because of their interesting mathematical and physical properties and their many possible applications.

**Nonlocal characteristic equations** The fundamental example is for a scalar \( \kappa = f \). The evolution of a scalar by (4) obeys

\[
\frac{\partial f}{\partial t} = \mathcal{L}_{(\delta E/\delta f)\mu[f]} \mu[f] = -\left( \frac{\delta E}{\delta f} \nabla \mu[f] \right) \cdot \nabla f.
\]

(7)

Equation (7) can be rewritten in characteristic form as \( df/dt = 0 \) on \( dx/dt = \left( \frac{\delta E}{\delta f} \nabla \mu[f] \right) \cdot \nabla f \). The characteristic speeds of this equation are **nonlocal** when \( \delta E/\delta f \) and \( \mu \) are chosen to depend on the average value, \( \bar{f} \).

One may verify that the scalar equation (7) admits weak solutions (5). Figure 1 shows the spatio-temporal numerical evolution of \( H \ast f \) given by (7) with initial conditions of the type
with \( \delta \)-functions whose strengths are random numbers between \( \pm 1/8 \). We have taken \( \delta E/\delta f = H \ast f \) where \( H \) is the inverse Helmholtz operator \( H(x) = e^{-|x|/\alpha} \) with \( \alpha = 1 \).

We see the evolution of sharp ridges in \( \tilde{f} = H \ast f \), which corresponds to \( \delta \)-functions in the solutions \( f(x,t) \).

Explicit equations for the evolution of strengths \( p_a \) and coordinates \( q_a \) for a sum of \( \delta \)-functions in (5) may be derived using (6) as

\[
\frac{\partial p_a(t,s)}{\partial t} = p_a(t,s) \text{div} \left( \frac{\delta E}{\delta f} \nabla \mu[f] \right)_{x=q_a(t,s)} \tag{8}
\]

\[
p_a(t,s) \frac{\partial q_a(t,s)}{\partial t} = p_a(t,s) \left( \frac{\delta E}{\delta f} \nabla \mu[f] \right)_{x=q_a(t,s)} \tag{9}
\]

for \( a = 1, 2, \ldots, N \). A solution containing a single \( \delta \)-function satisfies \( \dot{p} = -Ap^3 \), so an initial condition \( p(0) = p_0 \), evolves according to \( 1/p(t)^2 = 1/p_0^2 + 2At \). For the choice of our parameters in simulations, \( A = 2 \). The comparison of \( 1/p^2 \) from numerics with this theoretical prediction is shown in Figure 2.

We only mention that the evolution of a general 1-form (velocity) and 2-form (flux) may also be cast into the form of a nonlocal characteristic equation. For a 1-form in two- or three-dimensional space \( A \cdot dx \), the equation is quite complicated [10]. However, that equation allows a simplification in the case \( A = \nabla \psi \). The equation for potential \( \psi \) reads, with nonlocal \( \delta E/\delta \psi \) and \( \mu[\psi] \),

\[
\frac{\partial \psi}{\partial t} = \left( \frac{\delta E}{\delta \psi} \nabla \mu[\psi] \right)^\sharp \cdot \nabla \psi. \tag{10}
\]

This equation for the potential \( \psi \) has the same nonlocal characteristic structure as the scalar equation (7).

Similarly, the evolution of 2-form fluxes \( B \cdot dS = B_1 dx^2 \wedge dx^3 - B_2 dx^1 \wedge dx^3 + B_3 dx^1 \wedge dx^2 \) also simplifies. Again, the evolution for a general flux \( B \cdot dS \) is quite complicated, but it can be simplified for the case \( \text{div} B = 0 \) when \( B \) only depends on two coordinates \( (x,y) \). In this case, equation (11) may be written for the stream function \( \Psi \) in \( B = \text{curl} \tilde{\Psi} \hat{z} = \nabla \Psi \times \hat{z} \) as

\[
\frac{\partial \Psi}{\partial t} = \left( \frac{\delta E}{\delta \Psi} \nabla \Phi \right)^\sharp \cdot \nabla \Psi, \tag{11}
\]

when we choose mobility to be \( \mu = \text{curl} (\tilde{\Psi} \hat{z}) = \nabla \Phi \times \hat{z} \). Choosing \( \delta E/\delta \Psi \) and \( \Phi \) to depend on the average value \( \bar{\Psi} \) again yields a nonlocal characteristic equation.

**Nonlocal aggregation equations** Next, we consider the case which is the main focus of the paper, namely the orientation-dependent density. The evolution equations arising in this case are similar to (2) for mass density.
Density at each point is given by one number, whereas the number of coordinates necessary to describe the orientation by an element of the rotation group $SO(n)$ depends on the dimension of the space $n$. In two dimension, one number – turning angle – is enough, whereas in three dimensions three numbers are required. Keeping in spirit with the framework (11), we see that we cannot make a theory describing evolution of orientation per se, because $SO(n)$ is not a linear space. Instead, we need to consider the tangent space to $SO(n)$ taken at the identity, commonly denoted $so(n)$, which is a linear space. The description in terms of coordinates on $so(n)$ is simple and corresponds to physical intuition. So, let us define $\kappa$ to be a pair of densities $(\rho, \sigma)$ where $\rho$ is mass or number density and $\sigma$ is orientation density of particles, taking values in $so(n)$. Hence, we set $\kappa = \sum \kappa^a e_a$ where $e_a$ are basis vectors spanning the space of $\kappa$, $a = 0, 1, 2, 3$ with $a = 0$ corresponding to the mass density.

In 3-dimensional space, an elegant description of $\kappa$ exists using quaternions, obtained by associating the density part $a = 0$ with the scalar part and $a = 1, 2, 3$ with the ‘vector’ part of the quaternion. In two dimensions, an analogous description uses complex numbers. For orientation-dependent aggregation equation in 3D equation (11) reads

$$\frac{\partial \kappa^b}{\partial t} = - \text{div} \left( \mu^b [\kappa] \left( \kappa^a \nabla \frac{\delta E}{\delta \kappa^a} \right) \right), \quad a, b = 0, 1, 2, 3,$$

or, explicitly for $\rho$ and $\sigma^b$, $b = 1, 2, 3$:

$$\frac{\partial \rho}{\partial t} = - \text{div} \left( \mu^\rho \left( \rho \nabla \frac{\delta E}{\delta \rho} + \sigma^a \nabla \frac{\delta E}{\delta \sigma^a} \right) \right),$$

$$\frac{\partial \sigma^b}{\partial t} = - \text{div} \left( \mu^\sigma_b \left( \rho \nabla \frac{\delta E}{\delta \rho} + \sigma^a \nabla \frac{\delta E}{\delta \sigma^a} \right) \right).$$

(Summation on $a$ is assumed, but no summation on $b$.)

Interestingly enough, equations (13,14) allow weak solutions of the form (5). A special condition for existence of such solutions is that all mobilities $\mu^b$ must be constant along the flow. Then, even though ansatz (5) leads to an over-determined system, this system is consistent and for any real $K$, the following is an exact solution of (4,5):

$$p^b = K \mu^b [\kappa] \quad K \frac{\partial q^j}{\partial t} = \left( \rho^a \frac{\partial}{\partial x^j} \frac{\delta E}{\delta \kappa^a} \right)_{r=q(s,t)}.$$

In Figure 3, we present a simulation of the density and orientation in two dimensions. Starting with density and orientation spread unequally over two Gaussian ‘clumps’, we end up with a stationary solution whose density and orientation are concentrated into one clump. This is the nature of self assembly in this case.
Further developments  Equation (4) also encompasses ideal fluid vorticity dynamics (which is not associated with Darcy’s law). For the pairing $\langle \omega, m \rangle = \int \omega \cdot m \, dV$ between a divergenceless vector field $\omega = \omega \cdot \nabla$ and a one-form density $m = m \cdot dx \otimes dV$, set $\langle \frac{\partial \omega}{\partial t}, m \rangle = \langle \delta \omega, \frac{\delta E}{\delta \omega} \rangle$ and choose variation $\delta \omega = \mathcal{L}_{\text{curl} m} \omega = [\text{curl} m, \omega]$. After two integrations by parts, one finds $\frac{\partial}{\partial t} \omega = - [\text{curl} \frac{\delta E}{\delta \omega}, \omega]$ which recovers fluid vortex dynamics when $\text{curl} \frac{\delta E}{\delta \omega} = u$ and $\omega = \text{curl} u$. It will be interesting to see what other physical systems remain to be discovered in equation (4).

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Figure Captions.

Figure 1. Numerical simulation of scalar $f$, starting with initial condition which is a set of $\delta$-functions in $f$. The vertical coordinate represents $\overline{f} = H * f$, which remains finite even when $f$ forms $\delta$-functions, where $H(x) = e^{-|x|}$. The horizontal coordinate is space; the vertical coordinate is time.

Figure 2. Evolution of the $\delta$-function strength $1/p(t)^2$ versus time (circles). The theoretical prediction $1/p_0^2 + 4t$ is shown as a solid line obtained without any fitting parameters.

Figure 3. Numerical simulation of density $\rho$ starting with initial conditions for $\rho$ and $\sigma$ that are two Gaussian clumps of unequal strength $(\rho, \sigma)(r, 0) = \sum_{\text{clumps}}(\rho_0, \sigma_0) e^{-r^2/l_{\rho(\sigma)}^2}$. The initial conditions for $\rho$ and $\sigma$ are similar in shape but different in width. For this simulation, we have taken $l_\sigma = 2l_\rho$, $H(x) = e^{-|x|}$. Top: initial conditions, bottom: finite solution for $t = 30$. Left column: density, right column: orientation. White represents the domains of high density/orientation.
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