Mathematical Models for Self-Organization and Dissipation

Thanks to: Patrick Weidman (UC Boulder) 
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D.D.Holm, VP and C.Tronci, Physica D, submitted

Motivation: Directed Self-Assembly at Nano-Scales

Colloidal solution of 50nm particles deposited on a grooved substrate.

Water evaporates, contact line is pinned at grooves.

Particles dragged into the grooves and self-organize.
Application: **nano-sensors**

Small Resistance to electric current

Bio-agent is applied

Particles move

Large Resistance to electric current
Everything is self-assembly

It would be nice to figure out how Nature works:

Macro-scales I (many many km): Stars, galaxies *etc.*
Macro-scales II (many km-km): Clouds, river networks *etc.*
Macro-scales III (meters-cm): Forests, schools of fish *etc.*
Meso-scales IV (mm-100 microns): micro-devices, bugs *etc.*
Micro-scales V (microns- nanometers): nano-devices, proteins *etc.*

Macro-nano scales: Life on Earth
Self-assembly of round 2mm particles

t=0

t=5 min

t=10 min

t=20 min
Self-assembly of 4 mm stars
Round particles, Linear energy, singular solutions

Mathematical modeling framework:
Density is advected with velocity proportional to gradient of (potential of interaction, concentration of chemical ...)

Interacting particles + Diffusion:

Coagulation+Diffusion

Keller-Segel model of chemotaxis
More general than the models considered here: reduces to class discussed here in limiting cases

Self-Aggregation (swarming) of insects
Classical Debye-Huckel (etc) Equations

\[ \frac{\partial \rho}{\partial t} + \text{div} (\rho \mathbf{u}) = D \Delta \rho \quad \text{\( \mathbf{u} = \mu \text{grad} \Phi \)} \]

\[ \frac{\partial \Phi}{\partial t} + 0 = \Delta \Phi - \rho - \gamma \Phi \]

For particles of finite size, mobility can depend on density: at maximal density (1) mobility tends to zero

\[ \mu = 1 - \rho \]
Model proposed

\[
\frac{\partial \rho}{\partial t} + \text{div} (\rho \mathbf{u}) = D \Delta \bar{\rho} \quad \mathbf{u} = \mu(\bar{\rho}) \nabla \Phi
\]

Potential
\[
\Phi(x) = \int G(x - x') \rho(x') \, dx' = (G * \rho)(x)
\]

Averaged Density
\[
\bar{\rho}(x) = \int H(x - x') \rho(x') \, dx' = (H * \rho)(x)
\]

We use
\[
\mu(\bar{\rho}) = 1 - \bar{\rho} \quad \text{or} \quad \mu(\bar{\rho}) = 1
\]

Previous work: \( H(x) = \delta(x) \)

\( G(x) \) is inverse Laplacian or Helmholtz

Our work: \( H, G \) are nice functions

\[
G(x) = e^{-|x|/\alpha} \quad H(x) = \frac{1}{2\beta} e^{-|x|/\beta}
\]
Blow-up and regularity for positive mobility

Classical case: \( H(x) = \delta(x) \quad G(x) = \Delta^{-1} \)

One dimension: **no blow-up**, global bound in time for \( \rho \) in \( L^\infty \) and \( \Phi \) in \( W^{\sigma,p} \)


Two or more dimensions - **blow up** Brenner et al, *Nonlinearity* 12, 1071 (1999)

Are singularities bad? Look for

\[
\rho(x, t) = \sum_{j=1}^{N} w_j(t) \delta(x - q_j(t)) \]

\[
\bar{\rho}(x, t) = \sum_{j=1}^{N} w_j(t) H(x - q_j(t)) \]

A closed system of equations emerges

\[
\dot{w}_i(t) = 0 \quad \dot{q}_i(t) = -\sum_{j=1}^{N} w_j \mu(\bar{\rho}) G'(q_i - q_j) \]

\[
\begin{align*}
\text{Clumpons!}
\end{align*}
\]
Diffusion $D\Delta \bar{\rho}$ in our model does not prohibit formation of singularities, even in one dimension.

Note: Energy remains finite on delta-functions.

Clumpons!
What are stationary solutions for \( \mu(\bar{\rho}) = 1 - \bar{\rho} \)?

Particle velocity \( u = \mu(\bar{\rho}) \nabla \Phi = 0 \)

Two types of stationary solutions

- \( \Phi = \text{const} \)
- \( \bar{\rho} = 1 \)

Equilibrium Solutions | Jammed Solutions
---|---

Physically, we expect:

- **Unstable** (purely attractive force)
- **Stable**
Full numerical simulation starting with Gaussian initial conditions
Analytical solutions in two dimensions

Look for jammed solution with compact support

$$\bar{\rho} = H * \rho = 1$$  \hspace{1cm} \text{Linear equation!}

Analytical solutions for the case of inverse Helmholtz

An isolated patch with constant strength delta function at the boundary

2 D Helmholtz equation is separable in 4 cases (- cartesian)

<table>
<thead>
<tr>
<th>Polar coordinates</th>
<th>Circles</th>
<th>Bessel Functions</th>
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<tr>
<td>Elliptic Cylindrical</td>
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<tr>
<td>Elliptic Cylindrical</td>
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<td>Parabolae</td>
<td>Parabolic Cylinder Functions</td>
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</table>
Density Spectrum: Simulation vs Experiment

\[ \alpha = 1 \]
\[ \beta = 0.1 \]
\[ D = 0.01 \]

Theoretical model II: Non-central interaction

Need to consider density (scalar) + orientation (matrix in SO(3))

Now consider an arbitrary geometric quantity $\kappa(\mathbf{x}, t)$
We want to define equation of motion, based on Darcy’s law

velocity is proportional to force

so it reduces to Debye-Huckel equations when $\kappa(\mathbf{x}, t)$
is density (3-form).

But what is Darcy’s law for an arbitrary geometric quantity?
How do we express it for, say, 1-form densities, 2-forms,
density + orientation etc?
Mathematical Digression: Diamond and Gradient

Define a *pairing* \( \langle \cdot, \cdot \rangle \) (for *dual* things that can be multiplied and integrated, like scalars and 3-forms).

Then, define a *diamond* operator \( b \diamond a \) for dual objects \( a \) and \( b \) (it takes two dual objects and produces 1-form density): for any vector field \( \eta \)

\[
\langle b \diamond a , \eta \rangle \equiv - \langle b , \mathcal{L}_\eta a \rangle
\]

Diamond operator is antisymmetric: \( \langle b \diamond a + a \diamond b , \eta \rangle = 0 \)

Explicit examples of diamond operator - RHS multiplied by \( \cdot d\mathbf{x} \otimes d^3x \)

- \( f \) is a scalar \( f \diamond \frac{\delta E}{\delta f} = \frac{\delta E}{\delta f} \nabla f \)
- \( \mathbf{A} \cdot d\mathbf{x} \) is a one-form \( \mathbf{A} \diamond \frac{\delta E}{\delta \mathbf{A}} = \frac{\delta E}{\delta \mathbf{A}} \times \text{curl} \mathbf{A} - \mathbf{A} \text{div} \frac{\delta E}{\delta \mathbf{A}} \)
- \( \mathbf{B} \cdot dS \) is a two-form \( \mathbf{B} \diamond \frac{\delta E}{\delta \mathbf{B}} = \mathbf{B} \times \text{curl} \frac{\delta E}{\delta \mathbf{B}} - \frac{\delta E}{\delta \mathbf{B}} \text{div} \mathbf{B} \)
- \( D d^3x \) is a three-form \( D \diamond \frac{\delta E}{\delta D} = - D \nabla \frac{\delta E}{\delta D} \)

Let us also define operators relating of lowering and raising indices (no metric)

\[
(A \cdot d\mathbf{x} \otimes d^3x)^\# = A \cdot \frac{\partial}{\partial \mathbf{x}} \quad \quad \left( B \cdot \frac{\partial}{\partial \mathbf{x}} \right)^b = B \cdot d\mathbf{x} \otimes d^3x
\]
Motivating the answer

Density \( \rho d^n x \) (n-form) \[\begin{align*}
\frac{\partial \rho}{\partial t} &= -\text{div} (\rho u) \\
\frac{\partial \rho}{\partial t} &= - \mathcal{L} u \rho
\end{align*}\] Darcy’s velocity
\[u = \left( \mu \nabla \frac{\delta E}{\delta \rho} \right)^\#\] Final answer must be
\[\frac{\partial \kappa}{\partial t} = - \mathcal{L} \left( \mu \diamond \frac{\delta E}{\delta \kappa} \right)^\# \kappa \]

Arbitrary Geometric Quantity \( \kappa \) Mobility \( \mu \) is of the same type as \( \kappa \)
Simulation of Geometric Order Parameter (GOP) equation for orientation

2D simulation
Initial conditions are given by an isolated patch with random orientation.
Theorem [Energy dissipation]: Energy $E$ is evolving according to
\[
\frac{dE}{dt} = - \left\langle \left( \kappa \otimes \frac{\delta E}{\delta \kappa} \right), \left( \mu [\kappa] \otimes \frac{\delta E}{\delta \kappa} \right) \right\rangle
\]

Theorem [Existence of singular solutions-necessary conditions]: The weak form of the GOP equation contains only values and first derivatives of the arbitrary function so singular solutions may exist
\[
\left\langle \frac{\partial \kappa}{\partial t}, \phi \right\rangle = \left\langle - \mathcal{L} (\mu \otimes \frac{\delta E}{\delta \kappa})^\# \kappa, \phi \right\rangle = \left\langle \kappa \otimes \phi, (\mu \otimes \frac{\delta E}{\delta \kappa})^\# \right\rangle = \left\langle \kappa, \mathcal{L} (\mu \otimes \frac{\delta E}{\delta \kappa})^\# \phi \right\rangle
\]

Theorem [Collapse of singular solutions]: There exist initial conditions for scalar equation for which singular solutions collapse (merge) in finite time.

Simulation of two singular solutions with opposite amplitudes collapsing in finite time.
(Solid -theory, dashed-simulation)
Metric formulation

For an arbitrary functional $F$,

$$\frac{dF[\kappa]}{dt} = \left\langle \frac{\partial \kappa}{\partial t}, \frac{\delta F}{\delta \kappa} \right\rangle = \left\langle -\mathcal{L}_{(\mu[\kappa] \circ \frac{\delta E}{\delta \kappa})^\#}, \frac{\delta F}{\delta \kappa} \right\rangle$$

$$= -\left\langle \left(\mu[\kappa] \circ \frac{\delta E}{\delta \kappa}\right), \left(\kappa \circ \frac{\delta F}{\delta \kappa}\right)^\# \right\rangle =: \{\{E, F\}\}[\kappa]$$

defines *Metric Tensor* for any two functionals $F$ and $E$ and (as we see below) *Double Bracket (bracket of a bracket)*

Double Bracket comes from *Darcy’s law* (force proportional to velocity) so it is a way to introduce dissipation in a physical system - *Lie-Darcy’s dissipation*

Advantages:

1) Preserves coadjoint motion (modifying velocity) if added to inertia in the Euler-Poincare form
2) Allows singular solutions if mobility is nonlocal function
Connection to previous work

Double Bracket dissipation introduced before:
Bloch, Krishnaprasad, Marsden, Ratiu, Comm. Math. Phys, 175, 1-42 (1996);

Motivation: Dissipation in Euler equations and list sorting

Why not apply double bracket ideas to kinetic equations as a dissipation model?
Motivation: Mass-spectrometer using Atomic Force Microscope

Oscillating AFM tip creates particle dynamics
Possibility of separating particles (molecules) based on dynamical properties- Important to know dissipation
With Takashi Hikihara (Kyoto University, Engineering)

Mathematically:
Introducing dissipation into Vlasov’s equation for f(p,q,t)
For any two functionals E and F define (\{ , \}) is the Lie-Poisson bracket

\[
\{\{ E, F \} \} = - \left< \left< \mu[f], \frac{\delta E}{\delta f} \right>, \left< f, \frac{\delta F}{\delta f} \right> \right>
\]

Then for arbitrary functional F
dissipative dynamics is

\[
\frac{dF}{dt} = \{\{ E, F \} \}
\]

H. Kandrup, Astrophys. J. 380 511-514 (1991); \( \mu[f] = \alpha f \)
Dissipative Vlasov equation for particles with orientation

Suppose \( g \) is the space dual to the Lie algebra \( \mathfrak{so}(3) \) (or more general) Define a bracket as in Gibbons, Holm and Kuppershmidt, *Phys. Lett A*, **90**, 281-283 (1982); *ibid, Phys. D*, **6**, 179-194 (1982/3).  
\[
\{ f, h \}_1 := \{ f, h \} + \left\langle g, \left[ \frac{\partial f}{\partial g}, \frac{\partial h}{\partial g} \right] \right\rangle
\]
Taking moments & applying cold plasma closure yields *chromohydrodynamics*

The dissipative Vlasov equation is
\[
\frac{\partial f}{\partial t} = \left\{ f, \left\{ \mu[f], \frac{\delta E}{\delta f} \right\}_1 \right\}_1
\]

Equations of motion:
- \( \rho = \int f \, dg \, dp \)
- \( G = \int g \, f \, dg \, dp \)

Moments - Define
- \( \mu_{\rho} = \int \mu[f] \, dg \, dp \)
- \( \mu_{G} = \int g \, \mu[f] \, dg \, dp \)

Assume linearity in \( g \); Integrate with respect to \( p \) and \( g \)
Neglect all moments involving product \( pg \)
Truncate terms with moments (in \( p \)) higher than one

We obtain, at zeroth order -
\[
\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial q} \left( \rho \mu[\rho] \frac{\partial \delta E}{\partial \rho} \right)
\]
Evolution equations for density and orientation

\[
\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial q} \left( \rho \left( \mu_\rho \frac{\partial}{\partial q} \frac{\delta E}{\delta \rho} + \left\langle \mu_G, \frac{\partial}{\partial q} \frac{\delta E}{\delta G} \right\rangle \right) \right)
\]

\[
\frac{\partial G}{\partial t} = \frac{\partial}{\partial q} \left( G \left( \mu_\rho \frac{\partial}{\partial q} \frac{\delta E}{\delta \rho} + \left\langle \mu_G, \frac{\partial}{\partial q} \frac{\delta E}{\delta G} \right\rangle \right) \right) + \text{ad}^* \left( \text{ad}^* \frac{\delta E}{\delta G} \mu_G \right) \, \mathcal{G}.
\]

Diffusion

**Example: rod-like particles on a line - so(3) algebra**

\[ G = m(x), \quad \text{and} \quad \text{ad}_v^* w = -v \times w \quad \text{so} \]

\[
\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left( \rho \left( \mu_\rho \frac{\partial}{\partial x} \frac{\delta E}{\delta \rho} + \mu_m \cdot \frac{\partial}{\partial x} \frac{\delta E}{\delta m} \right) \right)
\]

\[
\frac{\partial m}{\partial t} = \frac{\partial}{\partial x} \left( m \left( \mu_\rho \frac{\partial}{\partial x} \frac{\delta E}{\delta \rho} + \mu_m \cdot \frac{\partial}{\partial x} \frac{\delta E}{\delta m} \right) \right) + m \times \mu_m \times \frac{\delta E}{\delta m}
\]

Gilbert dissipation for Landau-Lifschitz equation
Connection to Smoluchowski’s equation

Do not integrate with respect to $g$ 
$A_n(q, g) := \int p^n f(q, p, g) \, dp$

(only moments in $p$)

Use cold plasma approximation 
$A_2 = \frac{A_1^2}{A_0}$

\[
\frac{\partial A_0}{\partial t} = \frac{\partial}{\partial q} \left( A_0 F_{01} \right) + \frac{\partial}{\partial g} \cdot \left( A_0 \frac{\partial}{\partial g} \cdot (\hat{g} \, \lambda_0) - A_1 \frac{\partial}{\partial g} \cdot \hat{g} F_{01} \right)
\]

\[
\frac{\partial A_1}{\partial t} = \frac{\partial}{\partial q} \left( A_1 F_{01} \right) - A_0 \frac{\partial \lambda_1}{\partial q} + A_1 \frac{\partial}{\partial q} F_{01} + \frac{\partial}{\partial g} \cdot \left( A_1 \frac{\partial}{\partial g} \cdot (\hat{g} \, \lambda_0) - \frac{A_1^2}{A_0} \frac{\partial}{\partial g} \cdot (\hat{g} F_{01}) \right)
\]

Our variables $g$ are on Lie Algebra - not Lie group (2-sphere)
Compare with e.g. P. Constantin, Comm. Math. Sci, 3, 531-544 (2005)

\[
\frac{\partial A_0}{\partial t} = \partial_g \left[ \partial_g A_0 - A_0 \partial_g \left( G \ast A_0 \right) \right]
\]

Certain similarities are apparent but our tensors $\hat{g}$ are antisymmetric, so equations look different
Summary

1) We derived new equations for self-organizations of oriented particles from general conservation principles.
2) We suggested a dissipative Vlasov equation with the dissipation preserving weak solutions.
3) We derived a new dissipative equations for momenta - Lie-Darcy dissipation.
4) We suggested a kinetic origin of Gilbert dissipation in Landau-Lifshitz equations.

Future work

1) Study the appearance and dynamics of the generalized solutions to the new dissipative kinetic equations.
2) Study singular solutions in the new Lie-Darcy dissipative equations.
3) Applications to self-organization and protein dynamics.