Blowup Dynamics in the Keller-Segel Model of Chemotaxis

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To Evgeny Kusnetsov, with appreciation

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Chemotaxis

Chemotaxis is a directed movement of organisms in response to the concentration gradient of an external chemical signal and is common in biology.

The chemical signals either come from external sources or are secreted by the organisms themselves. The latter situation leads to aggregation of organisms and to the formation of patterns.

Chemotaxis underlies many social activities of micro-organisms, e.g. social motility, fruiting body development, quorum sensing and biofilm formation.

Chemotaxis: Examples

- Aggregation of bacteria (say, E. coli) under starvation conditions;
- Formation of multicellular structures of $\sim 10^5$ cells by single cell bacterivores, when challenged by adverse conditions;
- Formation of blood vessels.

Reduced Keller-Segel equations

Natural assumptions:
(a) the organism population is large and the individuals are small relative to the domain where they move
(b) the chemical diffuses much faster than the organisms do

$\Longrightarrow$ the simplest model of the gradient detection mechanism:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= \Delta \rho - \nabla \cdot (\rho \nabla c)\,, \\ 0 &= \Delta c + \rho. \end{aligned} \tag{1}$$

Here $\rho(x,t)$ and $c(x,t)$ are the organism density and chemical concentration.

Eq. (1) also appear in the context of

- stellar collapse
- non-Newtonian complex fluids
- crime patterns

Properties Keller-Segel equations

- Positivity preserv.: $\rho_0(x) \geq 0 \Longrightarrow \rho(x,t) \geq 0$ (max. pr.).
- Mass (number) conservation:

$$\int_\Omega \rho(x,t)\,dx = \int_\Omega \rho(x,0)\,dx.$$

- Scaling invariance: if a pair $\rho(x,t)$ and $c(x,t)$ is a solution to KS, then for any $\lambda > 0$ so is the pair

$$\lambda^{-2}\rho\left(\lambda^{-1}x, \lambda^{-2}t\right) \text{ and } c\left(\lambda^{-1}x, \lambda^{-2}t\right). \tag{2}$$

- Gradient property: $\partial_t \rho = -\mathrm{grad}\,\mathcal{F}(\rho)$, with the energy

$$\mathcal{F}(\rho) = \int_{\mathbb{R}^2} \left[-\frac{1}{2}\rho(-\Delta)^{-1}\rho + \rho \ln \rho \right] dx. \tag{3}$$

  and the metric $\langle v, w \rangle_J := \left\langle v, J^{-1}w \right\rangle_{L^2}$, $J := -\nabla \cdot \rho \nabla$.

Hence (a) $\mathcal{F}(\rho)$ decreases under the evolution and
(b) the critical points of $\mathcal{F}(\rho)$ are static solutions of KS.

Critical dimension

Under the scaling above, the total mass changes as

$$\int \frac{1}{\lambda^2}\rho\left(\frac{1}{\lambda}x,t\right)\,dx = \lambda^{(d-2)}\int \rho\left(x,t\right)\,dx.$$

One expects (a) global existence for $d=1$, (b) possible critical collapse for $d=2$ and (c) supercritical collapse for $d>2$.

For $d=2$, KS has a radially symmetric static solution (Wol, Vel):

$$R(x) := \frac{8}{(1+|x|^2)^2}, \tag{4}$$

and therefore, by the scaling invariance, the one-parameter family of radially symmetric static solutions,

$$R_\lambda(x) = \frac{1}{\lambda^2}R(\frac{1}{\lambda}x).$$

Key previous results

Consider the critical dimension $d = 2$. Recall, for $d = 2$, KS has a radially symmetric static solution, $R(x)$.

The total mass of R is $M = \int R(x) d^2x = 8\pi$. This mass turns out to be the threshold separating a regular behavior and a breakdown of the solution:

- (Blanchet, Dolbeault, Perthame) If the initial total mass satisfies $M := \int_{\mathbb{R}^2} \rho_0 \, dx \leq 8\pi$, then the solution to KS exists globally and, for $M := \int_{\mathbb{R}^2} \rho_0 \, dx < 8\pi$, converges to 0, as $t \to \infty$;
- (Biler) If the initial total mass satisfies $M := \int_{\mathbb{R}^2} \rho_0 \, dx > 8\pi$, then the solution to KS breaks down in finite time.

$M < 8\pi$: Existence argument

To investigate the long-time behaviour of KS, we follow Blanchet, Dolbeault, Perthame et al and compute the change in the entropy

$$\partial_t \int \rho \ln \rho = \underbrace{-4 \int |\nabla \sqrt{\rho}|^2}_{\text{entropy dissipation}} + \underbrace{\int \rho^2}_{\text{entropy production}} \quad .$$

Depending on whether the entropy dissipation or the entropy production wins we expect either dissipation or the collapse.

The Nirenberg - Gagliardo inequality (the dimension $n = 2$),

$$\int \rho^2 \leq c_{\mathrm{gn}} \int |\nabla \sqrt{\rho}|^2$$

shows the dissipation wins if $Mc_{\mathrm{gn}} < 4$ (here $M = \int \rho$).

$M < 8\pi$: Existence argument

To sharpen this result, one uses the logarithmic Hardy-Littlewood-Sobolev inequality (the dimension $n = 2$)

$$\mathcal{F}(\rho) \geq (\frac{1}{(M/8\pi)} - 1) \int \rho(-\Delta)^{-1}\rho - C(M), \tag{5}$$

where $M := \int \rho$ and $C(M) := M(1 + \log \pi - \log M)$. and that the free energy decreases, $\mathcal{F}(\rho) \leq \mathcal{F}(\rho_0)$, under the evolution to obtain the sharp entropy bound (Dolbeault, ...)

$$(1 - M/8\pi) \int \rho \log \rho \leq \mathcal{F}(\rho_0) - \frac{1}{4\pi} C(M),$$

which, in turn, leads the global existence for $M \leq 8\pi$.

To obtain the asymptotics of ρ one uses the more precise relation

$$\partial_t \mathcal{F}(\rho) = -\int \rho |\nabla \ln \rho - \nabla c|^2.$$

Virial relation

Differentiating the second moment, $W(t) := \int_{\mathbb{R}^2} x^2 \rho(x,t)\, dx$, of the density ρ, one arrives at the virial relation

$$\partial_t W = 4M(1 - \frac{1}{8\pi}M),$$

which shows how the mass threshold $M_* = 8\pi$ enters the dynamics:

If $M > 8\pi$, then the right hand side is constant and negative, and hence, W becomes negative in finite time $\Rightarrow$ contradiction, since $\rho(t) \geq 0$. Thus, if $M > 8\pi$, then the solution ρ breaks down in a finite time.

Our goal now is to investigate how this breakdown takes place.

$M > 8\pi$: Rescaling

Recall that KS has the manifold of static solutions

$$\mathcal{M}_{\rm stat} := \{\frac{1}{\lambda^2} R(x/\lambda) \mid \lambda > 0\}. \tag{6}$$

Assuming this manifold is stable, one can slide along it either in the direction $\lambda \to \infty$ (dissipation) or in the direction $\lambda \to 0$ (collapse).

To analyze the long time dynamics, we pass to the reference frame evolving (say, collapsing) with the solution, by introducing the *adaptive blowup variables*,

$$y = \frac{x}{\lambda(t)} \text{ and } \tau = \int_0^t \frac{1}{\lambda^2(s)}\, ds, \tag{7}$$

and $\lambda : [0, T) \to [0, \infty)$, $T > 0$ (*compression* or *dilatation* parameter), such that $\lambda(t) \to 0$ and $\tau \to \infty$, as $t \uparrow T$.

Rescaled Equation

The advantage of passing to blowup variables is that the function

$$u(y,\tau) = \lambda^2(t)\rho(x,t) \quad \text{with} \quad y = \frac{r}{\lambda(t)} \ \& \ \tau = \int_0^t \frac{1}{\lambda^2(s)}\, ds,$$

is expected to be *bounded* and the blowup time is eliminated from consideration: the new time $\tau \to \infty$ (it is mapped to ∞).

Writing KS in blowup variables and letting $v(y,\tau) = c(x,t)$, we find the equation for the rescaled bio mass density function

$$\partial_\tau u = \Delta_y u - \nabla \cdot (u \nabla v) - a \nabla_y \cdot (yu), \tag{8}$$

where $a := -\dot{\lambda}\lambda$. The blowup problem for KS is mapped into the problem of *asymptotic dynamics of solitons* for the equation (8).

Now, one can forget about λ and consider (8) as an equation for u and a and then find λ, by solving $-\dot{\lambda}\lambda = a$, given $\lambda(0) = \lambda_0$.

Stability analysis for $R(y)$

The rescaled KS involves two unknowns, u and a, and has the static solution $(R(y), a = 0)$.

To investigate stability of R, we linearize the rescaled KS around (R, a) $\Rightarrow$ the linear operator (cf. Wolansky)

$$L_a = -\Delta - \nabla \cdot \left((\nabla \Delta^{-1} R) + R \nabla \Delta^{-1} \right) + a \nabla \cdot y. \tag{9}$$

L_a is the hessian of the modified free energy functional

$$\mathcal{F}_a(u) = \int_{\mathbb{R}^2} \left[-\frac{1}{2} u(-\Delta)^{-1} u + u \ln u - \frac{a}{2} |y|^2 u \right] dx \tag{10}$$

at (R, a) and therefore it is self-adjoint in the inner product $\langle v, w \rangle_{J_R} := \langle v, J_R^{-1} w \rangle_{L^2}$, where $J_R := -\nabla \cdot R \nabla > 0$.

The operator L_a commutes with the rotations $\Longrightarrow$

$$L_a = \oplus_{m \geq 0} L_{am}.$$

Spectrum of the linearized map

DLOS have shown that L_{a0} (the radially symmetric part) has

- one negative eigenvalue $-2a + \frac{a}{\ln \frac{1}{a}} + O(a \ln^{-2} \frac{1}{a})$ (due to breaking of the scale covariance);
- one near zero eigenvalue (due to the shape instability);
- the third eigenvalue is $2a + \frac{2a}{\ln \frac{1}{a}} + O(a \ln^{-2} \frac{1}{a})$ (positive, but vanishing as $a \to 0$).

(The perturbation (adiabatic) parameter: $\frac{1}{\ln \frac{1}{a}}$.)

Dressing up the leading term

$\exists$ non-positive EVs $L_a \Rightarrow \mathcal{M}_{\rm stat} := \{\frac{1}{\lambda^2} R(x/\lambda) \mid \lambda > 0\}$ is unstable (with one unstable direction) and we have to construct a one-parameter deformation of it.

The simplest deformation of $R(y) := \frac{8}{(1+|y|^2)^2}$ is

$$R_{bc}(y) := \frac{8b}{(c+|y|^2)^2}, \qquad (11)$$

with $b > 1$, b and c close to 1 and with an extra relation between the parameters a, b and $c \Longrightarrow$
a two-param. family of approx. solutions to the rescaled KS $\Longrightarrow$
the deformation (or *almost center-unstable*) manifold

$$\mathcal{M}_{\text{stat deform}} := \{(1/\lambda^2) R_{bc}(x/\lambda) \mid \lambda > 0,\ b, c\}. \qquad (12)$$

This manifold absorbs all unstable/neutral degrees of freedom. The previous result gives the *linear stability* of $\mathcal{M}_{\text{stat deform}}$ in the *radially symmetric* case.

Splitting the solution

We expect that the solution to the rescaled KS approaches the manifold $\mathcal{M}_{\text{stat deform}}$, as $\tau \to \infty$.

Hence we decompose the solution $u(y,\tau)$ to the rescaled KS as

$$u(y,\tau) = \underbrace{R_{b(\tau)c(\tau)}(y)}_{\text{leading term, finite dim}} + \underbrace{\phi(y,\tau)}_{\text{fluctuation, infinite dim}}, \qquad (13)$$

and require that the fluctuation $\phi(y,\tau)$ is orthogonal to the tangent space of $\mathcal{M}_{\text{stat deform}}$ at $R_{b(\tau)c(\tau)}(y)$,

$$\langle \partial_{b,c} R_{b(\tau)c(\tau)}(\cdot), \phi(\cdot,\tau)\rangle = 0.$$

The leading term, $R_{b(\tau)c(\tau)}(y)$, and the fluctuation, $\phi(y,\tau)$, evolve on a *different spatial scales*, as R_{bc} can rewritten as

$$R_{bc}(y) = R_{\frac{b}{c^2},1}\left(\frac{y}{\sqrt{c}}\right).$$

Collapse dynamics

Restrict to the *radially symmetric* case. Substituting the splitting

$$u = R_{bc} + \phi$$

into the rescaled KS and projecting the resulting equation onto $\mathcal{M}_{\text{stat deform}}$, we arrive at

$$\begin{cases} c_\tau = 2a - \frac{4(b-1)}{\ln(\frac{1}{a})} + R_1(\phi, a, b, c), \\ \frac{b_\tau}{a} = -\frac{2(b-1)}{\ln(\frac{1}{a})} + R_2(\phi, a, b, c), \end{cases} \quad (14)$$

$|R_i(\phi, a, b, c)| \lesssim \frac{a}{\ln^2(\frac{1}{a})} \frac{1}{\ln(\frac{1}{a})}[(b-1)\|\phi\|_{L^2} + \|(1+|y|^2)^{-1}\phi\|_{L^2}^2],$
and an eqn for the fluctuation ϕ. To eliminate a large term on the r.h.s. we choose

$$b - 1 = \frac{1}{2} a \ln \frac{1}{a}.$$

then ignoring R_i, these equations give the differential eq. for a

$$a_\tau = -\frac{2a^2}{\ln(\frac{1}{a})} + O(\frac{a^2}{\ln^2(\frac{1}{a})}). \quad (15)$$

Solving the equation

$$a_\tau = -\frac{2a^2}{\ln(\frac{1}{a})} + O(\frac{a^2}{\ln^2(\frac{1}{a})}).$$

in the leading order and recalling that

$$\lambda(t)\dot{\lambda}(t) = -a(\tau)$$

where

$$\tau = \int_0^t \frac{1}{\lambda^2(s)}\, ds,$$

we obtain the scaling law

$$\lambda(t) = (T-t)^{\frac{1}{2}} e^{-|\frac{1}{2}\ln(T-t)|^{\frac{1}{2}}}(c_1 + o(1)).$$

Numerical simulations

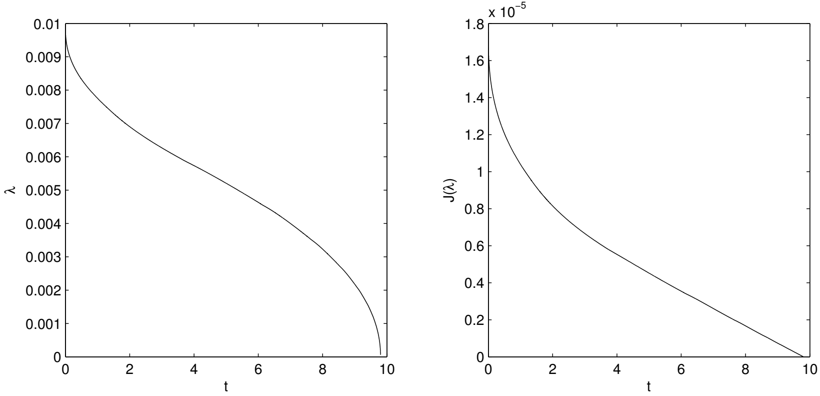

Figure: The right pane plots the quantity $J(\lambda) := e^{\sqrt{4 \ln \frac{\lambda_0}{\lambda}}} / \sqrt{\ln \frac{\lambda_0}{\lambda}} (\frac{\lambda}{\lambda_0})^2$ against time, which according to the $\lambda-$equation should be linear as the blowup time is approached.

Related Results and Conclusions

Related results: Velázquez, Herrero - Velázquez, Lushnikov, Dyachenko - Lushnikov - Vladimirova

Rigorous results: Rafael and Schweyer

Conclusions: We described the universal profile of the collapse, which depends in a 'self-similar' way on a single time-dependent parameter, λ, whose dynamics is is given by the equations

$$a_\tau = -\frac{2a^2}{\ln(\frac{1}{a})} + O(\frac{a^2}{\ln^2(\frac{1}{a})}), \tag{16}$$

$$\lambda(t)\dot{\lambda}(t) = -a(\tau(t)),$$

where the new and old times are related as $\tau = \tau(t) \equiv \int_0^t \frac{1}{\lambda^2(s)}\, ds$.

Perspectives

- Non-radially symmetric solutions
- The full Keller - Segel model
- Extension to many agents and to angiogenesis
- Kinetic and stochastic theory

  $$\partial_t f + v \cdot \nabla_x f = \lambda T f, \tag{17}$$

  where the LHS is the material derivative with $\dot{v} \cdot \nabla_x f$ neglected and $T = T(c)$ is a turning operator
- Incorporate intracellular chemosensory system
- Hyperbolic regimes
- Chemotaxis in self-generated fluid flow

Thank-you for your attention.

Comparison with Yang-Mills and Wave Maps Equations

Compare the dynamics for the scaling parameter $\lambda(t)$ for (MCF) and the critical Yang-Mills equation

$$\lambda\ddot{\lambda} = \frac{3}{4}\dot{\lambda}^4,$$

which gives

$$\lambda \approx \sqrt{\frac{2}{3}}\frac{t_* - t}{\sqrt{-\ln(t_* - t)}}.$$

and the critical wave map equation

$$\dot{\lambda}^2 = \lambda\ddot{\lambda}\ln\frac{a}{\lambda\ddot{\lambda}}\ , \ a = 0.122.$$