Infinite Time Aggregation for the Critical Patlak-Keller-Segel model in $\mathbb{R}^2$

Nader Masmoudi
Courant Institute of Mathematical Sciences,
New York University, NY 10012, U.S.A.
E-mail: masmoudi@cims.nyu.edu
http://www.math.nyu.edu/faculty/masmoudi/
Joint work with : A. Blanchet and J. Carrillo
Numerics : Paul Hand (CIMS).

Feb 9th 2007
Introduction
What is Chemotaxis?
Derivation of the Patlak-Keller-Segel model
Mathematical analysis
  A priori estimates
  Main results
  How does it blow-up?
  When does it blow-up?
  Does it blow-up at infinity?
Numerics
Conclusion
Introduction
The Patlak-Keller-Segel (PKS) model describes the collective motion of cells which are attracted by a self-emitted chemical substance. A model organism for this type of behavior is the *dictyostelium discoideum* which segregates cyclic adenosine monophosphate attracting themselves in starvation conditions. It is observed that after the appearance of a suitable number of mixamoebae, they aggregate to form a multi-cellular organism called pseudo-plasmoid.

C. S. Patlak (1953) and E. F. Keller and L. A. Segel (1970)
\[
\begin{aligned}
\frac{\partial n}{\partial t}(x, t) &= \Delta n(x, t) - \chi \nabla \cdot (n(x, t) \nabla c(x, t)) \\
\frac{\partial c}{\partial t}(x, t) &= \gamma c(x, t) - \tau c(x, t) = \nu \Delta c(x, t) + n(x, t), \\
n(x, t = 0) &= n_0 \geq 0,
\end{aligned}
\]

where \( x \in \mathbb{R}^2, \ t > 0 \). Here

- \((x, t) \mapsto n(x, t)\) represents the cell density, and
- \((x, t) \mapsto c(x, t)\) is the concentration of chemo-attractant.

The constant \( \chi > 0 \) is the sensitivity of the bacteria to the chemo-attractant.
The first equation takes into account that the motion of cells is driven by the steepest increase in the concentration of chemo-attractant while following a Brownian motion due to external interactions.

The second equation takes into account that cells are producing themselves the chemo-attractant while this is diffusing onto the environment. The time derivative of $c$ will be neglected assuming that the relaxation of the concentration is much quicker than the time scale of cell movement ($\gamma = \tau = 0, \nu = 1$).
What is Chemotaxis?

Chemotaxis is a kind of taxis, in which bodily cells, bacteria, and other single-cell or multicellular organisms direct their movements according to certain chemicals in their environment. This is important for bacteria to find food (for example, glucose) by swimming towards the highest concentration of food molecules, or to flee from poisons (for example, phenol).
Some bacteria, such as E. coli, have several flagella per cell (4-10 typically). These can rotate in two ways:

1. Counter-clockwise rotation aligns the flagella into a single rotating bundle, causing the bacterium to swim in a straight line.

2. Clockwise rotation breaks the flagella bundle apart such that each flagellum points in a different direction, causing the bacterium to tumble in place.
The overall movement of a bacterium is the result of alternating tumble and swim phases. It looks like a random walk with relatively straight swims interrupted by random tumbles that reorient the bacterium.

In the presence of a chemical gradient bacteria will chemotax: If the bacterium senses that it is moving in the correct direction (toward attractant), it will keep swimming in a straight line for longer before tumbling. If it is moving in the wrong direction, it will tumble sooner and try a new direction at random.

In other words, bacteria like E. coli use temporal sensing to decide whether life is getting better or worse.
Derivation of the Patlak-Keller-Segel model

There are
1) derivations from biased random walk models (Patlak 1953, Alt 1980, Othmer and Stevens 1997)
2) derivations from kinetic models
   Chalub, Markowich, B. Perthame, and C. Schmeiser 2004
\( f(t, x, v) \geq 0 \): phase space cell density

\[
\frac{\partial f}{\partial t}(t, x, v) + v \cdot \nabla_x f = \int_V (T[c]f' - T^*[c]f)dv'.
\]

where \( T[c] = T[c](t, x, v, v') \), \( T^*[c] = T[c](t, x, v', v) \) and \( f' = f(t, x, v') \).

In this model, it is assumed that the tumble (or reorientation) is a Poisson process with rate \( \lambda[c] = \int_V T^*[c]dv' \).

\( T^*[c]/\lambda[c] \) is the probability density for a change in velocity from \( v \) to \( v' \), given that a reorientation occurs for a cell at position \( x \), time \( t \) and velocity \( v \).
The PKS model can be derived by taking a parabolic scaling

\[
\frac{\partial f^\epsilon}{\partial t}(t, x, v) + \frac{1}{\epsilon} v \cdot \nabla_x f^\epsilon = \frac{1}{\epsilon^2} \int_V (T^\epsilon[c] f^{\epsilon'} - T^{\epsilon*}[c] f^\epsilon) dv'.
\]

where

\[
T^\epsilon[c] = T_0[c] + \epsilon T_1[c].
\]
The PKS system

\[
\begin{align*}
\frac{\partial n}{\partial t}(x, t) &= \Delta n(x, t) - \chi \nabla \cdot (n(x, t) \nabla c(x, t)) \\
-\Delta c(x, t) &= n(x, t) \\
n(x, t = 0) &= n_0 \geq 0
\end{align*}
\]  \hspace{1cm} (1)

where \(x \in \mathbb{R}^2\), \(t > 0\) and

\[
c(x, t) = -\frac{1}{2\pi} \int_{\mathbb{R}^2} \log |x - y| n(y, t) \, dy.
\]
The dimension 2 is critical when we consider the problem in $L^1$ because in $\mathbb{R}^2$ the Green kernel associated with $-\Delta c(x, t) = n(x, t)$ has a logarithmic singularity. In $\mathbb{R}^d$, for $d > 2$, the critical space is $L^{d/2}(\mathbb{R}^d)$.

In 1981, S. Childress and J. K. Percus conjectured in 2 dimensions that the aggregation or chemotactic collapse, if any, should proceed by the formation of a delta Dirac at the center of mass of cell density. Moreover, “the possibility of chemotactic collapse requires a threshold number of cells in the system”.

A priori estimates

Formal conservations of the total mass and center of mass

\[ M := \int_{\mathbb{R}^2} n_0(x) \, dx = \int_{\mathbb{R}^2} n(x, t) \, dx \]

\[ M_1 := \int_{\mathbb{R}^2} x n_0(x) \, dx = \int_{\mathbb{R}^2} x n(x, t) \, dx . \]

Moreover,

\[ \int_{\mathbb{R}^2} |x|^2 n(x, t) \, dx = \int_{\mathbb{R}^2} |x|^2 n_0(x) \, dx + 4M \left( 1 - \frac{\chi M}{8\pi} \right) t \]

There is a competition between the tendency of cells to spread all over \( \mathbb{R}^2 \) by diffusion and the tendency to aggregate because of the drift induced by the chemo-attractivity. The balance between these two mechanisms happens precisely at the critical mass \( \chi M = 8\pi \).
The critical case $\chi M = 8\pi$ has a family of explicit stationary solutions of the form

$$n_b(x) = \frac{8b}{\chi(b + |x|^2)^2}$$

with $b > 0$. All of these stationary solutions have critical mass and infinite second moment.
In the case $\chi M > 8\pi$, under the assumptions

$$\text{(H)} \quad (1 + |x|^2) n_0 \in L^1_+(\mathbb{R}^2) \quad \text{and} \quad n_0 \log n_0 \in L^1(\mathbb{R}^2).$$

on $n_0$, it is easy to see, using the second moment estimates, that global classical solutions to the Patlak-Keller-Segel system cannot exist and that they blow-up in finite time. Moreover, Herrero and Velázquez (96) constructed a solution such that

$$n(T^*) \sim \frac{8\pi}{\chi} \delta_{x=0} + \text{rest}.$$
Free energy functional:

\[ \mathcal{F}[n] = \int_{\mathbb{R}^2} n(x, t) \log n(x, t) \, dx - \frac{\chi}{2} \int_{\mathbb{R}^2} n(x, t) c(x, t) \, dx. \]

\[ = \int_{\mathbb{R}^2} n \log n \, dx + \frac{\chi}{4\pi} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} n(x) n(y) \log |x - y| \, dx \, dy. \]

Formally, we have

\[ \mathcal{F}[n](t) + \int_{0}^{t} \int_{\mathbb{R}^2} n(x, s) |\nabla (\log n(x))| - \chi \nabla c(x)|^2 \, dx \, ds = \mathcal{F}[n_0] \]
Theorem (Logarithmic Hardy-Littlewood-Sobolev inequality, Carlen-Loss, Beckner (93))

Let \( f \) be a non-negative function in \( L^1(\mathbb{R}^2) \) such that \( f \log f \) and \( f \log(1 + |x|^2) \) belong to \( L^1(\mathbb{R}^2) \). If \( \int_{\mathbb{R}^2} f \, dx = M \), then

\[
\int_{\mathbb{R}^2} f \log f \, dx + \frac{2}{M} \iint_{\mathbb{R}^4} f(x)f(y) \log |x - y| \, dx \, dy \geq - C(M),
\]

with \( C(M) := M(1 + \log \pi - \log M) \).
Some references:
Jäger and Luckhaus (92); Biler and Nadzieja (93)
Herrero and J. J. L. Velázquez (96)
Nagai, Senba and Yoshida (97), Senba and Suzuki
Horstmann (00), Gajewski and K. Zacharias
Brenner, Constantin, Kadanoff, Schenkel, Venkataramani (00)
Corrias, Perthame and Zaag (03), Dolbeault, Perthame (04)
Biler, Karch, Laurençot and Nadzieja (06)

Methods used: Best constant in Sobolev embeddings, energy methods, convolution estimates, Moser-Trudinger inequality, logarithmic Hardy-Littlewood-Sobolev inequality, asymptotic analysis....
Definition (Free-energy solution)

Given $T > 0$, the function $n$ is a free-energy solution to the Patlak-Keller-Segel system with initial data $n_0$ on $[0, T]$ if

$$\left(1 + |x|^2 + |\log n|\right) n \in L^\infty((0, T), L^1(\mathbb{R}^2)), \quad n \text{ satisfies the PKS system in the weak sense and}$$

$$\mathcal{F}[n](t) + \int_0^t \int_{\mathbb{R}^2} n(x, s) |\nabla (\log n(x)) - \chi \nabla c(x)|^2 \, dxds \leq \mathcal{F}[n_0]$$

for almost every $t \in (0, T)$. 
Main results

Theorem (Maximal Free-energy Solutions)

Under assumptions

\((H)\) \((1 + |x|^2) n_0 \in L^1_+ (\mathbb{R}^2) \) and \(n_0 \log n_0 \in L^1 (\mathbb{R}^2)\).

on the initial data \(n_0\), there exists a maximal time \(T^* > 0\) of existence of a free-energy solution to the PKS system

Moreover, if \(T^* < \infty\) then

\[
\lim_{t \uparrow T^*} \int_{\mathbb{R}^2} n(x, t) \log n(x, t) \ dx = +\infty.
\]
Theorem (Infinite Time Aggregation)

If $\chi M = 8\pi$, under assumptions

$$(H) \quad (1 + |x|^2) n_0 \in L^1_+ (\mathbb{R}^2) \quad \text{and} \quad n_0 \log n_0 \in L^1 (\mathbb{R}^2).$$

on the initial data $n_0$, there exists a global in time non-negative free-energy solution of the Patlak-Keller-Segel system with initial data $n_0$. Moreover if $\{t_p\}_{p \in \mathbb{N}} \to \infty$ as $p \to \infty$, then $t_p \mapsto n(x, t_p)$ converges to a delta Dirac of mass $8 \pi / \chi$ concentrated at the center of mass of the initial data weakly-* as measures as $p \to \infty$. 
Subcritical case $M < 8\pi/\chi$:

The entropy functional

$$S[n] = \int_{\mathbb{R}^2} n(x) \log n(x) \, dx.$$  

By the monotonicity of the free energy

$$\mathcal{F}[n] = (1-\theta)S[n] + \theta \left[ S[n] + \frac{\chi}{4\pi \theta} \iint_{\mathbb{R}^4} n(x) n(y) \log |x-y| \, dx \, dy \right]$$

is bounded from above by $\mathcal{F}[n_0]$. We choose $\theta = \frac{\chi M}{8\pi}$ and apply the Logarithmic Hardy-Littlewood-Sobolev inequality to get:

$$(1-\theta)S[n](t) - \theta C(M) \leq \mathcal{F}[n_0].$$

If $\chi M < 8\pi$, then $\theta < 1$ and

$$S[n](t) \leq \frac{\mathcal{F}[n_0] + \theta C(M)}{1-\theta}.$$
How does it blow-up?

Lemma (Characterization of Blowing-up Profile)

Under hypotheses (H) on the initial data, assume that $T^*$ the maximum time of existence of the free-energy solution $n$ to the Patlak-Keller-Segel system with initial data $n_0$ of critical mass $M = 8 \pi / \chi$ is finite. If $\{t_p\}_{p \in \mathbb{N}} \nearrow T^*$ when $p \to \infty$, then $t_p \mapsto n(x, t_p)$ converges to a delta Dirac of mass $8 \pi / \chi$ concentrated at the center of mass in the measure sense as $p \to \infty$. 
The main ideas of the proof reads as follows: We assume by contradiction that the weak-* limit of $t_p \mapsto n(x, t_p)$, namely $dn^*(x)$ is not a delta Dirac.

Hence, there exists a ball $B_{r_1}$ in which the mass of $dn^*$ is some $\alpha$ such that $0 < \alpha < M = 8 \pi / \chi$.

We also find a ball $B_{r_2}$, $r_2 > r_1$ such that the mass in $B_{r_2} \setminus B_{r_1}$ is small ($\leq 2\eta$).

We apply the Logarithmic Hardy-Littlewood-Sobolev inequality to some balls and annuli. By adding the corresponding terms, we obtain a uniform bound on the entropy $S[n](t_p)$. This contradicts the choice of the maximal time of existence.
Take $\rho = \frac{r_2 - r_1}{3}$. We apply the Logarithmic Hardy-Littlewood-Sobolev inequality to $n_\rho(x) := n(x, t_\rho)$ on the sets $B_{r_1 + \rho}$, $B_{r_2 - \rho}^c$ and $B_{r_2} \setminus B_{r_1}$ for $p$ large enough to obtain
\[
\int_{B_{r_1+\rho}} n_p \int_{B_{r_1+\rho}} n_p \log n_p + 2 \int\int_{B_{r_1+\rho} \times B_{r_1+\rho}} n_p(x) n_p(y) \log |x - y| \, dx \, dy \geq C_{r_1, \rho}
\]

\[
\int_{B_{r_2-\rho}^c} n_p \int_{B_{r_2-\rho}^c} n_p \log n_p + 2 \int\int_{B_{r_2-\rho}^c \times B_{r_2-\rho}^c} n_p(x) n_p(y) \log |x - y| \, dx \, dy \geq C_{r_2, \rho}
\]

\[
\int_{B_{r_2} \setminus B_{r_1}} n_p \int_{B_{r_2} \setminus B_{r_1}} n_p \log n_p + 2 \int\int_{B_{r_2} \setminus B_{r_1} \times B_{r_2} \setminus B_{r_1}} n_p(x) n_p(y) \log |x - y| \, dx \, dy \geq C_{r_1, r_2}
\]

We expand \( n \log n = n \log^+ n - n \log^- n \) in the first terms and disregard the negative part contribution. Using

\( B_{r_1+\rho} = B_{r_1} \cup S_1, \quad B_{r_2-\rho}^c = B_{r_2}^c \cup S_2, \quad \text{and} \quad B_{r_2} \setminus B_{r_1} = S_1 \cup S_2 \cup S_3 \)

adding the terms and collecting terms to reconstruct the integral in the whole \( \mathbb{R}^2 \) of the positive contribution of the entropy, we deduce
\[ \mathcal{K}_p \int_{\mathbb{R}^2} n_p \log^+ n_p + 2 \iint_{\mathbb{R}^2 \times \mathbb{R}^2} n_p(x) n_p(y) \log |x - y| \, dx \, dy \]
\[ - 4 \iint_{[B_{r_1} \times B_{r_1}^c] \cup [(S_1 \cup S_3) \times B_{r_2}^c]} n_p(x)n_p(y) \log |x - y| \, dx \, dy \]
\[ + 2 \iint_{[S_1 \times S_1] \cup [S_2 \times S_2]} n_p(x)n_p(y) \log |x - y| \, dx \, dy \geq C \]

with

\[ \mathcal{K}_p := \max \{ a_1, a_1 + a_2, a_2, a_2 + a_3, a_3 \} = \max \{ a_1 + a_2, a_2 + a_3 \}, \]

and

\[ a_1 := \int_{B_{r_1 + \rho}} n_p, \quad a_2 := \int_{(B_{r_2} \setminus B_{r_1})} n_p, \quad a_3 := \int_{B_{r_2 - \rho}^c} n_p(x) \, dx, \]
Finally, we get

$$\mathcal{K} \int_{\mathbb{R}^2} n_p \log n_p \, dx + 2 \int \int_{\mathbb{R}^2 \times \mathbb{R}^2} n_p(x) n_p(y) \log |x - y| \, dx \, dy \geq C$$

for $p$ big enough with $0 < \mathcal{K} < \frac{8\pi}{\chi}$.

Repeating the same arguments as in the subcritical case, and using the estimate on the free energy, we deduce

$$S[n_p] \leq \frac{\mathcal{F}[n_0] + \theta \, C(M)}{1 - \theta}.$$

with $\theta = \frac{\chi \mathcal{K}}{8\pi}$, for all $p$ big enough.

This fact contradicts the choice of $T^*$ as the maximal time of existence of a free-energy solution.
When does it blow-up?

Theorem (Existence of global in time solution)

Under assumptions \((H)\) on the initial data \(n_0\), there exists a nonnegative free-energy solution \(n\) to the Patlak-Keller-Segel system on \([0, \infty)\).

First, notice that there exists \(\Phi_0\) convex satisfying

\[
\lim_{r \to \infty} \frac{\Phi_0(r)}{r} = \infty \quad \text{and such that}
\]

\[
\int_{\mathbb{R}^2} \Phi_0(|x|^2) n(x, t) \, dx.
\]

A simple computation shows that

\[
\int_{\mathbb{R}^2} \Phi_0(|x|^2) n(x, t) \, dx \leq e^{c_1 t} \left[ \int_{\mathbb{R}^2} \Phi_0(|x|^2) n_0(x) \, dx + \frac{4c_2 M}{c_1} \right]
\]
Assume by contradiction that $T^* < \infty$. We first recall that in the case $\chi M = 8 \pi$, the second-momentum of a free-energy solution to the Patlak-Keller-Segel system is conserved,

$$\int_{\mathbb{R}^2} |x|^2 n_0(x) \, dx = \int_{\mathbb{R}^2} |x|^2 n(x, t) \, dx > 0. \quad (2)$$

Let us take $\{t_p\}_{p \in \mathbb{N}} \nearrow T^*$. Due to the tail-control, we get the tightness of the densities $\{|x|^2 n(x, t_p)\}_{p \in \mathbb{N}}$ in $\mathcal{M}(\mathbb{R}^2)$. As a conclusion, the sequence of densities $\{n(x, t_p)\}_{p \in \mathbb{N}}$ converges weakly-\ast as measures towards $dn^* \in \mathcal{M}(\mathbb{R}^2)$ with

$$\int_{\mathbb{R}^2} |x|^2 \, dn^*(x) = \int_{\mathbb{R}^2} |x|^2 n_0(x) \, dx > 0, \quad (3)$$

contradicting the fact that $dn^*$ should coincide with $M \delta_0$.
Does it blow-up at infinity?

Lemma (Blow-up at infinite time)

Under assumptions (H) on the initial data \( n_0 \), given any free-energy solution \( n \) of PKS system, we have

\[
\lim_{t \to \infty} n(t) = \frac{8 \pi}{\chi} \delta_{M_1} \text{ weakly-* as measures.}
\]

Proof: Assume by contradiction the existence of an increasing sequence of times \( \{t_p\}_{p \in \mathbb{N}} \uparrow \infty \) for which

\[
S[n_p] = \int_{\mathbb{R}^2} n(x, t_p) \log n(x, t_p) \, dx
\]

is bounded. Then, the Fisher information is integrable and

\[
\lim_{t \to \infty} \int_t^\infty \left( \int_{\mathbb{R}^2} n(x, s) \left| \nabla \log n(x, s) - \chi \nabla c(x, s) \right|^2 \, dx \right) \, ds = 0,
\]
which shows that, up to the extraction of sub-sequences, the limit $n_\infty(s, x)$ of $(s, x) \mapsto n(x, t + s)$ when $t$ goes to infinity satisfies

$$
\nabla \log n_\infty - \chi \nabla c_\infty = 0 , \quad c_\infty = -\frac{1}{2\pi} \log |\cdot| * n_\infty ,
$$

this is equivalent to the fact that $(n_\infty, c_\infty)$ solves the nonlocal nonlinear elliptic equation

$$
n_\infty = M \frac{e^{\chi c_\infty}}{\int_{\mathbb{R}^2} e^{\chi c_\infty} \, dx} = -\Delta c_\infty , \quad \text{with} \quad c_\infty = -\frac{1}{2\pi} \log |\cdot| * n_\infty .
$$

Moreover, by Chen, and Li (91), the solutions are radially symmetric. In the case $\chi M = 8\pi$, these are the family of radial stationary solutions $n_b$ defined earlier. For all $b$, the stationary solutions $n_b$ have infinite second momentum contradicting the conservation of the second momentum.
Long time behavior in the subcritical case $M < 8\pi/\chi$

$$\|n - n_\infty\|_{L^1} + \|\nabla c - \nabla c_\infty\|_{L^2} \to 0 \text{ when } t \to \infty$$

where

$$n_\infty(t, x) = \frac{1}{1 + 2t} u_\infty(x/\sqrt{1 + 2t}),$$

$$c_\infty(t, x) = v_\infty(x/\sqrt{1 + 2t}),$$

$$u_\infty = M \frac{e^\chi v_\infty - |x|^2/2}{\int_{\mathbb{R}^2} e^\chi v_\infty - |x|^2/2 \, dx} \quad \text{with} \quad v_\infty = -\frac{1}{2\pi} \log |\cdot| \ast u_\infty.$$
Time Evolution — Mass 7.9 Pi

Max vs. Time
Conclusion

Several questions are not very well understood:

- Time asymptotics, rate of convergence, speed of blow up
- The bounded domain case and domains with corners
- Kinetic models
- Derivation of hyperbolic models which may explain the formation of networks.