Stochastic Particle Approximation to the Keller-Segel Model in 2D

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The Keller-Segel model of chemotaxis

The **(Patlak (1953))-Keller-Segel (1970)** model describing the self-induced chemotactic movement of cells on the macroscopic level:

- cell density ϱ
- concentration of the chemical S

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\partial_t \varrho + \nabla \cdot (\varrho \chi \nabla S - \nabla \varrho) &= 0\,, \qquad \chi := 1\,, \\
-\Delta S &= \varrho\,,
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subject to $\varrho(x, t = 0) = \varrho_0(x)\,, \qquad x \in \mathbb{R}^2$

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Poisson equation $\rightsquigarrow$ 2D Newtonian potential:

$$S[\varrho](x,t) = -\frac{1}{2\pi} \int_{\mathbb{R}^2} \log|x-y| \varrho(y,t)\,\mathrm{d}y\,.$$

Dichotomy in 2D

Formal evolution of the 2nd order moment:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^2}\varrho(x)\frac{|x|^2}{2}\,\mathrm{d}x = \frac{M}{2\pi}(8\pi - M) \qquad \text{with } M = \int_{\mathbb{R}^2}\varrho(x)\,\mathrm{d}x\,.$$

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Theorem [Jäger-Luckhaus, 1992], [Blanchet-Dolbeault-Perthame, 2006]:

- Let $(1 + |x|^2 + \log\varrho)\varrho(t=0) \in L^1(\mathbb{R}^2)$
- Then
  - a) $M < 8\pi \rightsquigarrow$ global existence
  - b) $M > 8\pi \rightsquigarrow$ blow-up in finite time
  - c) $M = 8\pi \rightsquigarrow$ blow-up for $t \to \infty$ [Blanchet-Carrillo-Masmoudi, 2007]

What happens after blow-up?

- Regularization of the 2D Newtonian potential:

$$S_\varepsilon[\varrho](x) = -\frac{1}{2\pi}\int_{\mathbb{R}^2} \log(|x-y|+\varepsilon)\,\varrho(y)\,\mathrm{d}y \qquad \text{with } \varepsilon > 0$$

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- Limit $\varepsilon \to 0$ [Dolbeault-Schmeiser, 2008]:

$$\partial_t \varrho + \nabla \cdot (j[\varrho,\nu] - \nabla \varrho) = 0$$

with
  - a global weak solution $\varrho(t) \in \mathcal{M}_1^+(\mathbb{R}^2)$,
  - defect measure $\nu(t) \in \mathcal{M}(\mathbb{R}^2)^{\otimes 2}$,
  - and flux $j = j[\varrho,\nu]$.

Strong formulation after blow-up

Ansatz: smooth part + finite number of singularities:

$$\varrho(x,t) = \bar{\varrho}(x,t) + \sum_{n \in \mathcal{S}} M_n(t)\delta(x - x_n(t))\,.$$

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Then

$$M_n \geq 8\pi \text{ for all } n \in \mathcal{S}$$

and

$$\partial_t\bar\varrho + \nabla\cdot(\bar\varrho\nabla S[\bar\varrho] - \nabla\bar\varrho) - \frac{1}{2\pi}\nabla\bar\varrho\cdot\sum_{n\in\mathcal{S}} M_n(t)\frac{x - x_n}{|x - x_n|^2} = 0$$

$$\dot M_n = M_n\bar\varrho(x = x_n)$$

$$\dot x_n = \nabla S[\bar\varrho](x = x_n) - \frac{1}{2\pi}\sum_{m\neq n} M_m\frac{x_n - x_m}{|x_n - x_m|^2}$$

... locally in time [Velazquez'04].

Numerics

- Numerical solution *in the smooth regime:*
  [Filbet'06]: finite volumes
  [Morrocco'03]: mixed finite elements
  [Saito-Suzuki'05,'07]: finite differences
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- Our approach: Stochastic particle approximation

$$\bar{\varrho}(x,t) \approx \sum_{n \in \mathcal{R}} M_n(t) \delta(x - x_n(t))$$

driven by the SDE

$$\mathrm{d}x_n = -\frac{1}{2\pi} \sum_{m \neq n} M_m \frac{x_n - x_m}{|x_n - x_m|^2} \,\mathrm{d}t + \sqrt{2}\,\mathrm{d}B_t^n \,.$$

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- Movement of the singular particles $(n \in \mathcal{S})$:

$$\dot{x}_n = -\frac{1}{2\pi}\sum_{m\neq n} M_m \frac{x_n - x_m}{|x_n - x_m|^2}\,\mathrm{d}t\,.$$

Dynamical analysis

Define the discrete total mass and 2nd order moment:

$$M = \sum_{n \in \mathcal{R} \cup \mathcal{S}} M_n \,, \qquad u(t) = \sum_{n \in \mathcal{R} \cup \mathcal{S}} M_n \frac{|x_n(t)|^2}{2} \,.$$

Formal application of the Itô-calculus, with only regular particles, gives

$$\frac{\mathrm{d}}{\mathrm{d}t} E[u(t)] = \left(M^2 - \sum_{n \in \mathcal{R}} M_n^2 \right) \left(-\frac{1}{2\pi} + \frac{4}{M} \right) .$$

$\leadsto$ critical mass 8π.

Implementation

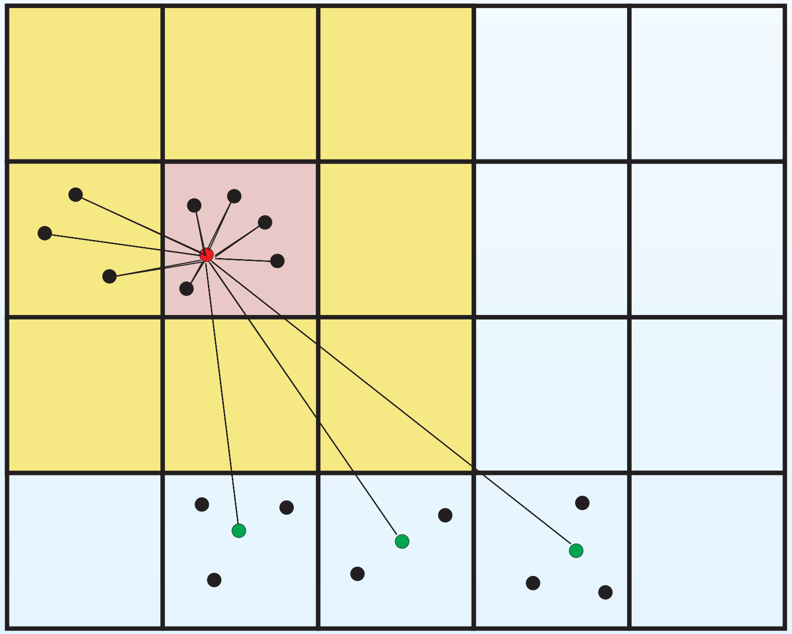
- Discretization in time: Euler-Maruyama method.
- Collision of M and m iff $|\Delta x|^2 \leq \Delta t \frac{M+m}{2\pi}$.
  - Ensures stability of the algorithm ($\sim$ CFL)
  - Leads to the correct dynamics: $\dot{M}_n = M_n \bar{\varrho}(x = x_n)$.
- Splitting of randomly chosen *regular* particles:
  - The total number of particles is conserved.
  - Good resolution of $\bar{\varrho}$.
- Blow-up detection: Creation of a particle with mass $\geq 8\pi$.

Technical issues

... how to accelerate the $O(N^2)$ algorithm?

Localization of particles:

- Near particles - exact computation
- Far particles - approximation using particle clustering



For huge ensembles: Fast multipole method - $O(N \log N)$, $O(N)$

The algorithm

- Particle interactions:
  - Clustering & Computation of centers of gravity
  - Evaluation of particle interactions:

    Near interactions: Particle-Particle

    Far interactions: Particle-Cluster
- Collisions, splitting
- Blow-up detection
- Brownian motion

Convergence

The Fokker-Planck equation for $p^N = p^N(t; x_1, \ldots, x_N)$ corresponding to the system of N indistinguishable particles with mass M/N and with the regularized interaction kernel:

$$\frac{\partial p^N}{\partial t} + \sum_{n=1}^{N} \nabla_{x_n} \cdot \left[-\frac{1}{2\pi} \frac{M}{N} \sum_{m \neq n} \mathcal{K}^\varepsilon (x_n - x_m) p^N - \nabla_{x_n} p^N \right] = 0 \,,$$

$$L^\infty \ni \mathcal{K}^\varepsilon(z) := \frac{z}{|z|(|z| + \varepsilon)} \qquad \text{for } z \in \mathbb{R}^2 \,.$$

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$(\varepsilon > 0,\ N < \infty)$	$\longrightarrow_{N\to\infty}$	$(K-S)_{\varepsilon > 0}$
$\downarrow_{\varepsilon \to 0}$		$\downarrow_{\varepsilon \to 0}$
“sticky particles”	$\longrightarrow_{N\to\infty}$	$(K-S)$

Simple limit: $\varepsilon > 0$ fixed, $N \to \infty$

- BBGKY hierarchy for k-particle marginals, $k = 1, \ldots, N$:

$$P_k^N(t, x_1, \ldots, x_k) := \int_{\mathbb{R}^{2(N-k)}} p^N(t, x_1, \ldots, x_N)\, \mathrm{d}x_{k+1} \ldots \mathrm{d}x_N \,.$$

- Boltzmann hierarchy for $P_k := \lim_{N\to\infty} P_k^N$.

Theorem. The Boltzmann hierarchy has *unique* solutions

$$P_k(t, x_1, \ldots, x_k) = \prod_{i=1}^{k} P_1(t, x_i) \qquad \forall k \geq 2\,,$$

with $\varrho(t,x) := M P_1(t,x)$ a solution to the regularized Keller-Segel system.

Tough limit: $\varepsilon \to 0$, then $N \to \infty$

- Technical toolbox:
  - BBGKY hierarchy, marginals
  - Tight convergence, defect measures for the interaction terms

$$\int_{\mathbb{R}^{2k}} \frac{x_n - x_m}{|x_n - x_m|(|x_n - x_m| + \varepsilon)} P_k^{\varepsilon,N} \cdot (\nabla_{x_n} - \nabla_{x_m})\varphi \, \mathrm{d}x$$

- Tight boundedness of $P_k^{\varepsilon,N}$ uniformly in ε and N; consequently:
  - $P_k^{\varepsilon,N} \rightharpoonup (P_k^N, \nu_k^N)$ when $\varepsilon \to 0$
  - $(P_k^N, \nu_k^N) \rightharpoonup (P_k, \nu_k)$ when $N \to \infty$

  in the sense of tight convergence of measures.

Tough limit: $\varepsilon \to 0$, then $N \to \infty$

- The Boltzmann hierarchy *admits* the molecular chaos solution

$$P_k(t,x_1,\dots,x_k) = \prod_{i=1}^{k} P_1(t,x_i)\,,$$

$$\nu_k(t;y;x_2,\dots,x_k) = \nu_1(t,y)\prod_{i=2}^{k} P_1(t,x_i)$$

where

$$(\varrho,\nu) := (MP_1, M^2\nu_1)$$

satisfies the weak formulation of the Keller-Segel system.

- But, no hope for uniqueness of P_k
  $\Rightarrow$ only the *"compatibility result"* possible.

The limit $\varepsilon \to 0$: Two particles

- Fokker-Planck for $p^\varepsilon = p^\varepsilon(t, x, y)$, $x, y \in \mathbb{R}^2$,

$$\frac{\partial p^\varepsilon}{\partial t} - \frac{M}{4\pi}(\nabla_x - \nabla_y) \cdot j^\varepsilon - (\Delta_x + \Delta_y)p^\varepsilon = 0\,,$$

with

$$j^\varepsilon(x, y) = \frac{x - y}{|x - y|(|x - y| + \varepsilon)} p^\varepsilon(x, y)\,,$$

subject to the symmetric initial condition

$$p^\varepsilon(t = 0, x, y) = p_I(x, y) = p_I(y, x)$$

The limit $\varepsilon \longrightarrow 0$: Two particles

- Tight boundedness of $\{p^\varepsilon\}_{\varepsilon>0} \rightsquigarrow$

$$p^\varepsilon \longrightarrow p \qquad \text{tightly as } \varepsilon \longrightarrow 0\,.$$

- Weak formulation of the limiting interaction term:

$$\frac{M}{4\pi}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}\frac{x-y}{|x-y|^2}p\cdot(\nabla_x-\nabla_y)\varphi(x,y)\,\mathrm{d}x\,\mathrm{d}y$$
$$+\frac{1}{2}\frac{M}{4\pi}\int_{\mathbb{R}^2}\nu(x):(\nabla_x-\nabla_y)^{\otimes 2}\varphi(x,x)\,\mathrm{d}x\,,$$

with $\nu(x)$ symmetric, nonnegative and

$$\mathrm{tr}(\nu(x)) \le p(x,\{x\}) := \int_{\mathbb{R}^2} p(x,y)\chi(x-y)\,\mathrm{d}y\,.$$

The limit $\varepsilon \to 0$: Two particles

Two blow-up scenarios for p:

- $M < 8\pi$: L^∞-blow-up at $x = y$, but no concentration:

$$\frac{\partial p}{\partial t} - \frac{M}{4\pi}(\nabla_x - \nabla_y) \cdot j - (\Delta_x + \Delta_y)p = 0\,,$$

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- $M > 8\pi$: concentration blow-up at $x = y$:

$$p(t, x, y) = p_0(t, x, y) + p_1(t, x)\delta(x - y) \qquad \text{with } p_0, p_1 \text{ smooth}$$

governed by

$$\begin{aligned} \frac{\partial p_0}{\partial t} - \frac{M}{4\pi}\frac{x-y}{|x-y|^2} \cdot (\nabla_x - \nabla_y)p_0 - (\Delta_x + \Delta_y)p_0 &= 0 \\ \frac{\partial p_1}{\partial t} - \frac{1}{2}\Delta_x p_1 &= \frac{M}{4}p_0(x, x) \end{aligned}$$

A general rule

It is a concurrence of two effects:

- Interaction (attraction)
  - pushing the particles together
  - with strength proportional to M
- Diffusion
  - pulling the particles apart
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General rule:

An aggregate of particles is stable if and only if its mass is greater than 8π

Three particles

Possible configurations:

- 3 free particles
- 1 pair + 1 free particle
- 1 triplet

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Possible scenarios:

- $M < 8\pi$: particles collide, but do not stick together
- $8\pi < M < 12\pi$: ?? (only the aggregate of three particles can be stable)
- $M > 12\pi$: also pairs of particles are stable

Conclusions

Thank you for your attention!