Particle Systems for Keller-Segel equations

with
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The Keller-Segel equation (1970)

Cells diffuse in $\mathbb{R}^2$ and are attracted by a chemical substance that they deposit. This substance also diffuses in the plane.

$$\partial_t \rho_t(x) = \Delta \rho_t(x) - \chi \,\mathrm{div}\left[\rho_t(x) \nabla c_t(x)\right],$$

$$\theta\, \partial_t c_t(x) = \Delta c_t(x) + \rho_t(x).$$

$\rho_t(x) \geq 0$: density of cells at $x \in \mathbb{R}^2$ at time $t \geq 0$ (with mass 1).

$c_t(x) \geq 0$: concentration of substance at $x \in \mathbb{R}^2$ at time $t \geq 0$.

$\chi > 0$: intensity of the attraction.

$\theta \geq 0$: ratio between the diffusion velocities of cells and substance.

I. The parabolic-elliptic case $\theta = 0$

The substance diffuses very quickly, but the cells deposit a lot of substance. For each fixed $t \geq 0$, we solve $0 = \Delta c_t(x) + \rho_t(x)$:

$$c_t(x) = -(K \star \rho_t)(x), \quad \text{where} \quad K(x) = \frac{\log |x|^2}{4\pi}, \quad \text{so} \quad \nabla K(x) = \frac{x}{2\pi |x|^2}.$$

The KS equation (parabolic-elliptic) is rewritten as

$$\partial_t \rho_t(x) = \Delta \rho_t(x) + \chi \mathrm{div} \left[\rho_t(x) (\nabla K \star \rho_t)(x) \right].$$

We can forget about the substance: the cells diffuse in the plane $\mathbb{R}^2$ and interact through a binary attraction in $1/r$.

Strong competition between diffusion and attraction in $1/r$: we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^2}|x|^2\rho_t(x)\mathrm{d}x = 4 - \frac{\chi}{2\pi}.$$

- If $\chi > 8\pi$, no global existence is possible. Formation of a Dirac mass in finite time: attraction is stronger than diffusion.

- Global existence if $\chi < 8\pi$: Blanchet-Dolbeault-Perthame (2006). Use the optimal constant of the logarithmic Hardy-Littlewood-Sobolev inequality.

Particle System

Approximation of the equation by the particle system in $(\mathbb{R}^2)^N$

$$\mathrm{d}X_t^{i,N} = \sqrt{2}\mathrm{d}B_t^i - \frac{\chi}{2\pi N}\sum_{j\neq i}\frac{X_t^{i,N}-X_t^{j,N}}{|X_t^{i,N}-X_t^{j,N}|^2}\mathrm{d}t, \qquad i=1,\dots,N.$$

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Theorem (F-Jourdain, F-Tardy, Tardy)
If $\chi \in (0, 8\pi)$, then the particle system exists for each N, with only (but effectively) binary collisions, and if $\mu_0^N \to \rho_0 \in \mathcal{P}(\mathbb{R}^2)$ and under exchangeability, then $(\mu_t^N)_{t\geq 0}$ converges, up to extraction of a subsequence, to a (very weak) solution ρ_t of KS.

- No assumption on $\rho_0 \in \mathcal{P}(\mathbb{R}^2)$, Dirac allowed, diffusion immediately separates the particles.

- $\theta = 8\pi$ also works (if $\rho_0 \neq \delta$), more difficult, in particular because the particle system explodes for each N, but later and later as $N \to \infty$.

- Bresch-Jabin-Wang (2023).

- Cattiaux-Pédèches (2016), Cattiaux (2024).

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The main difficulty is to show that for some $\gamma > 0$, uniformly in N,

$$\sup_{N\geq 2} \mathbb{E}\Big[\int_0^T \frac{\mathrm{d}t}{|X_t^{1,N} - X_t^{2,N}|^\gamma} \mathrm{d}t\Big] < \infty \qquad \text{for all } T > 0.$$

The rest of the proof is standard.

Consider $\alpha \in (0,2)$, and we compute (with $X_t^i := X_t^{i,N}$)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}[|X_t^1 - X_t^2|^\alpha] = 4\alpha^2\mathbb{E}[|X_t^1 - X_t^2|^{\alpha-2}] - \frac{\alpha\chi}{2\pi}I_t,$$

where, by exchangeability,

$$\begin{aligned} I_t =& \mathbb{E}\Big[|X_t^1 - X_t^2|^{\alpha-2}(X_t^1 - X_t^2) \cdot \Big(\frac{X_t^1 - X_t^3}{|X_t^1 - X_t^3|^2} - \frac{X_t^2 - X_t^3}{|X_t^2 - X_t^3|^2}\Big)\Big] \\ =& \frac{1}{3}\mathbb{E}[F(X_t^1, X_t^2, X_t^3)], \end{aligned}$$

with

$$\begin{aligned} F(x,y,z) =& |x-y|^{\alpha-2}(x-y) \cdot \Big(\frac{x-z}{|x-z|^2} - \frac{y-z}{|y-z|^2}\Big) \\ &+ |y-z|^{\alpha-2}(y-z) \cdot \Big(\frac{y-x}{|y-x|^2} - \frac{z-x}{|z-x|^2}\Big) \\ &+ |z-x|^{\alpha-2}(z-x) \cdot \Big(\frac{z-y}{|z-y|^2} - \frac{x-y}{|x-y|^2}\Big) \\ \le& |x-y|^{\alpha-2} + |y-z|^{\alpha-2} + |z-x|^{\alpha-2} \end{aligned}$$

by a simple function study.

So

$$I_t \leq \frac{1}{3}\mathbb{E}[|X_t^1-X_t^2|^{\alpha-2}+|X_t^2-X_t^3|^{\alpha-2}+|X_t^3-X_t^1|^{\alpha-2}] = \mathbb{E}[|X_t^1-X_t^2|^{\alpha-2}],$$

then

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}[|X_t^1 - X_t^2|^\alpha] \geq \Big(4\alpha^2 - \frac{\alpha\chi}{2\pi}\Big)\mathbb{E}[|X_t^1 - X_t^2|^{\alpha-2}].$$

If $\chi < 8\pi$, we can find $\alpha \in (0,2)$ such that $4\alpha^2 > \frac{\alpha\chi}{2\pi}$. Thus

$$\int_0^T \mathbb{E}[|X_t^1 - X_t^2|^{\alpha-2}]\mathrm{d}t \leq C_{\alpha,\chi}\mathbb{E}[|X_T^1 - X_T^2|^\alpha] \leq C_{\alpha,\chi,T} \qquad \forall T > 0,$$

at least if we assume $\mathbb{E}[|X_0^1|^\alpha] < \infty$. Since $\alpha - 2 < 0$, OK.

We can remove the moment assumption $\mathbb{E}[|X_0^1|^\alpha] < \infty$.

The same computation gives a new (very simple) proof of global existence for the KS equation with $\chi < 8\pi$.

II. Supercritical parabolic-elliptic case $\chi > 8\pi$

We fix $N \geq 2$ and study the explosion of the system

$$\mathrm{d}X_t^i = \sqrt{2}\mathrm{d}B_t^i - \frac{\chi}{2\pi N}\sum_{j\neq i}\frac{X_t^i - X_t^j}{|X_t^i - X_t^j|^2}\mathrm{d}t, \qquad i = 1, \dots, N.$$

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A Bessel process with dimension $\delta \in \mathbb{R}$ is the solution $R_t \geq 0$ of

$$R_t = R_0 + W_t + \frac{\delta - 1}{2} \int_0^t \frac{\mathrm{d}s}{R_s} \qquad \text{(a bit false if } \delta \leq 1).$$

If $\delta \in \mathbb{N}_*$, it is the norm of a Brownian of dimension δ. Perfect competition between diffusion and attraction/repulsion (by 0) in $1/r$:

- if $\delta \geq 2$, $R_t > 0$ for all $t > 0$;
- if $\delta \in (0, 2)$, R_t touches uncountably 0 many times;
- if $\delta \leq 0$, R_t touches 0 and cannot restart.

Assume that our system $(X_t^1, ..., X_t^N)_{t \geq 0}$ exists.

- A simple Itô calculation shows that

$$\sum_{i,j=1}^{N} |X_t^i - X_t^j|^2$$

is a (square of) Bessel with dimension $(N-1)(2-\frac{\chi}{4\pi})$ (negative if $\chi \geq 8\pi$).

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- ▶ Let $K \subset \{1, \dots, N\}$. When particles indexed in K are "far" from particles indexed in K^c, we can neglect interactions between K and K^c. We find that

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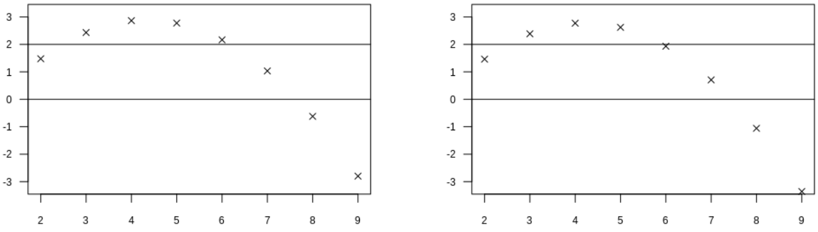
- Of course, $\sum_{i,j\in K} |X_t^i - X_t^j|^2$ touches 0 if and only if particles indexed in K collide.

Figure: $d_{\chi,N}(k)$ as a function of $k \in [\![2, N]\!]$ when $N = 9$ and $\chi = 9.4\pi$ (left) or $\chi = 9.68\pi$ (right).



$k_0 = 8,\ k_1 = 7$

$k_0 = 8,\ k_1 = 7,\ k_2 = 6$

$k_0 = \lceil 8\pi N/\chi \rceil$ is the smallest integer such that $d_{\chi,N}(k) \leq 0$.

We always have $d_{\chi,N}(k_0 - 1) \in (0, 2)$. We set $k_1 = k_0 - 1$.

Sometimes, $d_{\chi,N}(k_0 - 2) \in (0, 2)$, then we set $k_2 = k_0 - 2$.

Sometimes $d_{\chi,N}(k_0 - 2) \geq 2$.

We always have $d_{\chi,N}(2) \in (0, 2)$ and $d_{\chi,N}(k) \geq 2$ for $k = 3, \dots, k_0 - 3$.

So, we believe there should be non-sticky collisions with $2, k_2, k_1$ particles, sticky (explosive) collisions with k_0 (or more) particles, and no collisions with $3, \ldots, k_0 - 3$ particles.

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Existence of the system: we use Fukushima's theory of Dirichlet forms. The invariant measure of the system, on $(\mathbb{R}^2)^N$, which is informally

$$\Big(\prod_{i \neq j} |x_i - x_j|^{-\chi/(4\pi N)}\Big) \mathrm{d}x_1 \dots \mathrm{d}x_N,$$

is Radon (finite on compacts) precisely on the open set

$$E_{k_0} = \{\text{no cluster of } k_0 \text{ (or more) particles}\} \subset (\mathbb{R}^2)^N.$$

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Fukushima provides us for free a solution $X_t = (X_t^1, \ldots, X_t^N)_{t \in [0,\zeta)}$, in a (very) weak sense, up to "explosion" ζ, meaning exit from (any compact of) E_{k_0}.

Theorem (with Tardy). Assume $\chi \geq 8\pi$ and $N > 12\pi\chi$. We have $k_0 = \lceil 2N/\theta \rceil \in \{7, ..., N\}$, we set $k_1 = k_0 - 1$, and $k_2 = k_0 - 2$ *(or no k_2)*.

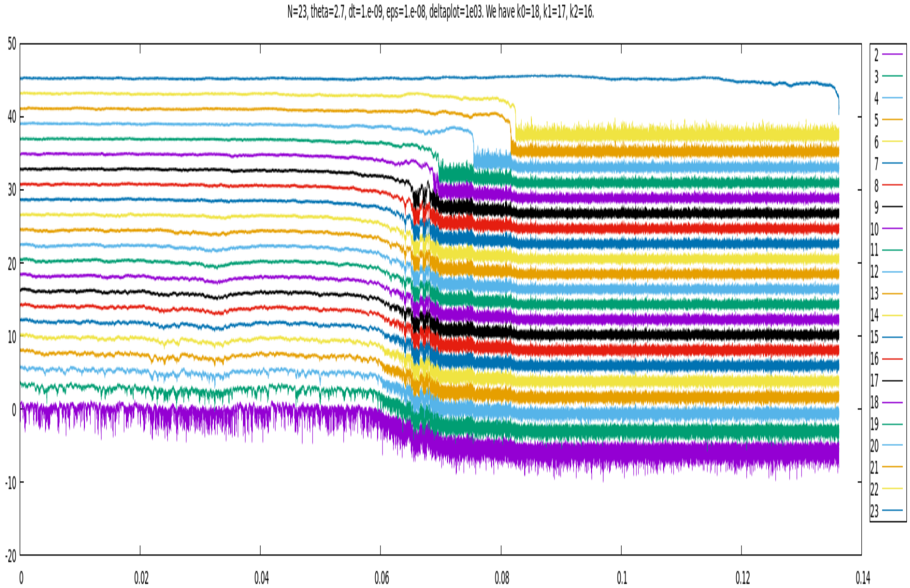
(i) $\zeta < \infty$ and $\lim_{t \to \zeta-} X_t$ exists in $(\mathbb{R}^2)^N$ and contains a cluster of precisely k_0 particles, indexed in a random $K_0 \subset \{1, ..., N\}$.

(ii) Just before ζ, we have uncountably many collisions of any subset of K_0 with cardinal k_1.

(iii) Before each k_1-collision, we have uncountably many k_2-collisions of all possible configurations.

(iv) Before each k_2-collision, we have uncountably many 2-collisions of all possible configurations.

(v) There are no collisions with precisely $3, \ldots, k_2 - 1$ particles.



N=23, theta=2.7, dt=1.e-09, eps=1.e-08, deltaplot=1e03. We have k0=18, k1=17, k2=16.

III. The parabolic-parabolic case $\theta > 0$

Regarding the PDE, the main results are

- Calvez-Corrias (2008): global existence, for any $\theta > 0$, and any $\chi < 8\pi$ (if ρ_0, c_0 are regular).
- Corrias-Escobedo-Matos (2014): if $c_0 = 0$, global existence for any $\chi < \chi_\theta$, with $\chi_\theta \to \infty$ as $\theta \to \infty$ (if ρ_0 is regular).
- Mizoguchi (2020): if $\chi > 8\pi$, there exist initial conditions (c_0, ρ_0) such that the solution blows up.

One-species particle system, Talay-Tomašević (2017)

We solve $\theta\partial_t c_t = \Delta c_t + \rho_t$ (taking $c_0 = 0$ for simplicity):

$$c_t = \frac{1}{\theta}\int_0^t g^\theta_{t-s} \star \rho_s \;\; \mathrm{d}s, \quad \text{where} \quad g^\theta_t = \mathcal{N}\Big(0, \frac{t}{\theta} I_2\Big).$$

Recall that

$$\partial_t \rho_t = \Delta\rho_t - \chi \mathrm{div}(\rho_t \nabla c_t).$$

A possible (non-Markovian) particle system: for $i = 1, \ldots, N$,

$$\mathrm{d}X^{i,N}_t = \sqrt{2}\mathrm{d}B^i_t + \frac{\chi}{N}\sum_{j\neq i}\Big(\frac{1}{\theta}\int_0^t \nabla g^\theta_{t-s}(X^{i,N}_t - X^{j,N}_s)\mathrm{d}s\Big)\mathrm{d}t.$$

Theorem (with Tomašević 2023). For each $\theta > 0$, there exists $\chi_\theta > 0$ such that if $\chi < \chi_\theta$, then

(a) for each $N \geq 2$, the system has a solution (for any exchangeable initial condition),

(b) if $\mu_0^N \to \rho_0$, then, up to a subsequence, $(\mu_t^N = \frac{1}{N}\sum_{i=1}^N \delta_{X_t^{i,N}})_{t\geq 0}$ converges to (very weak) a solution $(\rho_t)_{t\geq 0}$ of Keller-Segel.

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- We assume that $\rho_0 \in \mathcal{P}(\mathbb{R}^2)$ and $c_0 \in L^\infty(\mathbb{R}^2)$.
- The threshold χ_θ does not depend on (ρ_0, c_0).
- $\chi_{\theta=0.0001} \simeq 3.28$, $\chi_{\theta=1} \simeq 1.39$, $\chi_\theta \sim \frac{1.65}{\sqrt{\theta}}$ as $\theta \to \infty$ (much smaller than 8π).

Proof ideas, with e.g., $\theta = 1$. We denote $g_t = g_t^\theta$ and $X_t^i = X_t^{i,N}$.

The difficulty is to control, uniformly in N, the drift, e.g.

$$D_t^{12} = \int_0^t \nabla g_{t-s}(X_t^1 - X_s^2)\mathrm{d}s \simeq \int_0^t e^{\frac{-|X_t^1 - X_s^2|^2}{t-s}} \frac{X_t^1 - X_s^2}{(t-s)^2}\mathrm{d}s.$$

We show **using the dynamics** that *a priori*,

$$|D_t^{12}| \lesssim |X_t^1 - X_t^2|^{-1} \qquad \text{in a weak sense.}$$

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Precisely, we show that there exist $\alpha > 1$ and C (independent of $t > 0$, $N \geq 2$, and $\chi > 0$ small) such that

$$\mathbb{E}\Big[\int_0^t |D_s^{12}|^\alpha \mathrm{d}s\Big] \leq C\mathbb{E}\Big[\int_0^t \frac{\mathrm{d}s}{|X_s^1 - X_s^2|^\alpha}\Big].$$

(a) For $F : \mathbb{R}_+ \times \mathbb{R}^2 \to \mathbb{R}$,

$$\begin{aligned}\mathbb{E}\Big[\int_0^t F(t-s, X_t^1 - X_s^2)\mathrm{d}s\Big] = \mathbb{E}\Big[\int_0^t F(0, X_s^1 - X_s^2)\mathrm{d}s\Big] \\ + \mathbb{E}\Big[\int_0^t \int_0^u (\partial_t F + \Delta F)(u-s, X_u^1 - X_s^2)\mathrm{d}u\mathrm{d}s\Big] \\ + \chi\mathbb{E}\Big[\int_0^t D_s^{13} \cdot \Big(\int_0^s \nabla F(u-s, X_u^1 - X_s^2)\mathrm{d}u\Big)\mathrm{d}s\Big].\end{aligned}$$

We start with ($t > s$)

$$X_t^1 - X_s^2 = X_s^1 - X_s^2 + B_t^1 - B_s^1 + \frac{1}{N}\sum_{j=2}^{N}\int_s^t D_u^{1j}\mathrm{d}u,$$

we apply Itô in t, with s fixed, to calculate $F(t-s, X_t^1 - X_s^2)$. We integrate over $s \in [0,t]$, take the expectation, and use exchangeability.

(b) We have $|\nabla g_t(x)| \le \frac{C}{(t+|x|^2)^{3/2}}$ (*sharp* when $|x|^2 \simeq t$), and thus

$$|D_s^{13}| \le C\int_0^s (s-u+|X_s^1 - X_u^3|^2)^{-3/2}\mathrm{d}u.$$

(c) Let $F(t,x) = -(t+|x|^2)^{-\frac{\alpha}{2}}$ for $\alpha \in (1,2)$. We have

$$(\partial_t F + \Delta F)(t,x) \geq c(t+|x|^2)^{-1-\frac{\alpha}{2}} \quad \text{and} \quad |\nabla F(t,x)| \leq C(t+|x|^2)^{-\frac{1}{2}-\frac{\alpha}{2}}.$$

(d) We use this F in (a), and obtain

$$(\text{negative}) = -\mathbb{E}\Big[\int_0^t |X_s^1 - X_s^2|^{-\alpha} \mathrm{d}s\Big] + I_t + J_t,$$

where

$$\begin{aligned} I_t \geq & c\mathbb{E}\Big[\int_0^t \int_0^s (s-u+|X_s^1 - X_u^2|^2)^{-1-\frac{\alpha}{2}} \mathrm{d}u\mathrm{d}s\Big] \\ |J_t| \leq & \chi C\mathbb{E}\Big[\int_0^t |D_s^{13}|\Big(\int_0^s (s-u+|X_s^1 - X_u^2|^2)^{-\frac{1}{2}-\frac{\alpha}{2}} \mathrm{d}u\Big)\mathrm{d}s\Big]. \end{aligned}$$

(e) By (b) and a sort of "Hölder inequality", $|J_t| \leq \chi C I_t$, then

$$(1-\chi C) I_t \leq \mathbb{E}\Big[\int_0^t |X_s^1 - X_s^2|^{-\alpha} \mathrm{d}s\Big].$$

(f) By (b) and a "Hölder inequality", $\int_0^t (D_s^{12})^\alpha \mathrm{d}s \leq C I_t$. So if $\chi < 1/(2C)$,

$$\mathbb{E}\Big[\int_0^t (D_s^{12})^\alpha \mathrm{d}s\Big] \leq C I_t \leq C\mathbb{E}\Big[\int_0^t |X_s^1 - X_s^2|^{-\alpha} \mathrm{d}s\Big].$$

"Hölder inequality". For all $b > a > 0$, all $s \geq 0$, all $f : [0, s] \to \mathbb{R}_+$,

$$\int_0^s \frac{\mathrm{d}u}{(u + f(u))^{1+a}} \leq \kappa_{a,b} \Big[\int_0^s \frac{\mathrm{d}u}{(u + f(u))^{1+b}} \Big]^{a/b},$$

and the optimal constant is (for all $s \geq 0$)

$$\kappa_{a,b} = \frac{a+1}{a} \Big[\frac{b}{b+1} \Big]^{a/b}$$

(quasi-saturated by $f_\epsilon(u) = (\epsilon - u)_+$).

Thanks to Calvez and Perthame.

Two-species particle system, Stevens (2000)

We assume $c_0 = 0$ for simplicity. Fix $N \geq 2$ and a real $M > 0$. We have N cells and a varying number of chemical particles.

- Initially, the N cell positions are i.i.d. and ρ_0-distributed, and we have no chemical particles.

- Each cell produces chemical particles according to a Poisson process with rate $\theta^{-1}M$. When a chemical particle is born, it takes the position of its mother cell.

- Each chemical particle moves like a Brownian motion with diffusion coefficient $\sqrt{2\theta^{-1}}$.

- The i-th cell moves like a Brownian motion with diffusion coefficient $\sqrt{2}$ and drifts according to

$$(\nabla \phi_\epsilon * \nu_t^i)(X_t^i),$$

where ϕ_ϵ is a mollifier and where ν_t^i is the empirical concentration at time t of chemical particles, excluding those produced by the i-th cell and normalized by $M(N-1)$.

With Tomašević (in progress), we can show, with a similar but more involved proof, that if $\chi < \chi_\theta$ (same value for χ_θ),

(i) for N fixed, as $M \to \infty$, and $\epsilon = \epsilon_M \to 0$ such that $\lim_M M\epsilon_M^{3+} = \infty$, the two-species particle system tends (up to extraction) to the one-species particle system;

(ii) as $N \to \infty$, with $M = M_N$ and $\epsilon = \epsilon_N \to 0$ s.t. $\lim_N NM_N\epsilon_N^{3+} = \infty$, the two-species particle system approximates (up to extraction) the KS equation.

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- In (ii), M_N may tend to 0, the important point is that $NM_N \to \infty$.
- Maybe (?) we would be happier with 3+ replaced by 2.
- Stevens (2000) shows a true convergence to the KS equation, for all χ, θ such that the KS equation has a unique smooth solution, under the conditions $M_N = 1$ and $\lim_N N\epsilon_N^{15+} = \infty$.

Thank You