Applications of Coalescing Interacting Particles to Chemotaxis Models

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End Goal

For N particles in $\mathbb{R}^2$ with

$$dX_t^{(n)} = -\chi \frac{\partial}{\partial X_t^{(n)}} \sum_{\substack{i=1 \\ i \neq n}}^{N} m_i V(X_t^{(n)}, X_t^{(i)}) dt + \sqrt{\frac{2\tilde{\mu}}{m_n}} dW_t^{(n)} \tag{1}$$

and V is a logarithmically singular potential, we want to:

- Investigate inelastic collisions
- Look at hydrodynamic limits
- Simulate system

And apply the above to:

- Solving the Keller-Segel system and other PDEs pre- and post-blow-up

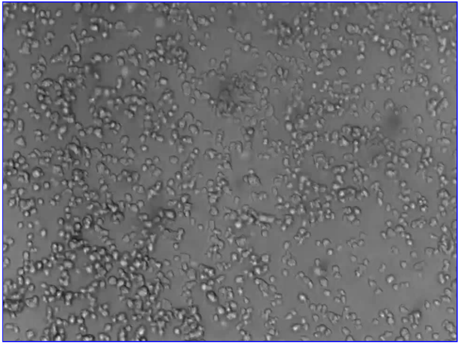
Overview

- Motivation
- Keller-Segel model and blow-up
- Particle systems and inelastic collisions
- Simulation of particle systems
- Particle method for solving regularized PDEs
- Multispecies K-S as a limit of nonuniform particles
- Blow-up in multispecies K-S

Motivation...

& General Overview

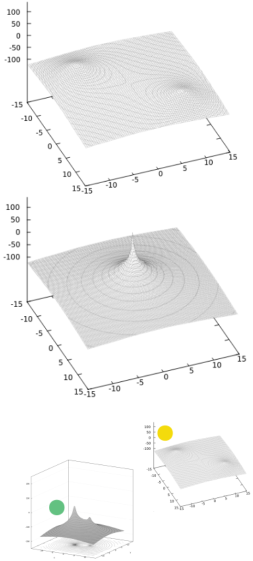
Aggregation of the Social Amoeba



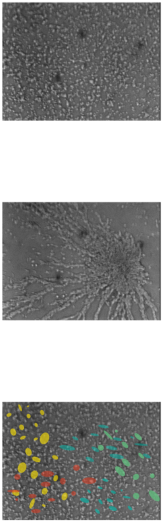
(Vijay Ramani, Laboratory for the Physics of Life , Department of Physics, Princeton University.)

- $3 \rightarrow 18$ hours post-starvation
- 1947: John Bonner discovers above emergent behavior *when there are enough cells*
- Each amoeba leaves a chemical attractant trail
- Cells drift in the direction of most chemoattractant

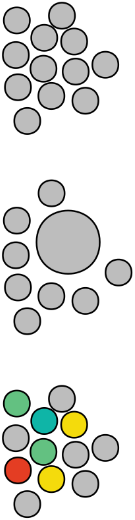
Contiuum model



THE REAL WORLD

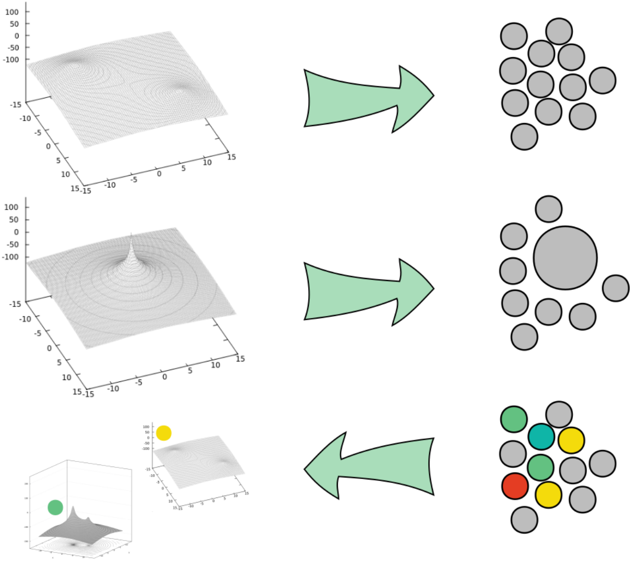


Particle model



Contiuum model

Particle model



The Keller-Segel Model

Keller-Segel model

- 1970: Evelyn Keller and Lee Segel introduce K-S system[1] [5] for modeling aggregation in $\mathbb{R}^2$:

$$\begin{cases} \partial_t \rho(x,t) & = \nabla \cdot (\mu \nabla \rho - \chi \rho \nabla c) \\ \partial_t c(x,t) & = \Delta c - k^2 c + \rho \end{cases} \tag{2}$$

- $c(x,t)$—chemoattractant concentration
- $\rho(x,t)$—cell density, with

$$\int \rho(x,t)dx = M < \infty \text{—constant total mass} \tag{3}$$

- μ—mobility of particles, χ—chemosensitivity

[1] Independently introduced by Patlak in 1952 with applications to long-chain polymers [7].

KELLER-SEGEL MODEL

- 1970: Evelyn Keller and Lee Segel introduce K-S system[2] [5] for modeling aggregation in $\mathbb{R}^2$:

$$\begin{cases} \partial_t \rho(x,t) & = \nabla \cdot (\mu \nabla \rho - \chi \rho \nabla c) \\ 0 & = \Delta c - 0c + \rho \end{cases} \tag{4}$$

- $c(x,t)$—chemoattractant concentration
- $\rho(x,t)$—cell density, with

$$\int \rho(x,t)dx = M < \infty \text{—constant total mass} \tag{5}$$

- μ—mobility of particles, χ—chemosensitivity

[2] Independently introduced by Patlak in 1952 with applications to long-chain polymers [7].

KELLER-SEGEL MODEL (ELLIPTIC)

- 1970: Evelyn Keller and Lee Segel introduce K-S system[3] [5] for modeling aggregation in $\mathbb{R}^2$:

$$\begin{cases} \partial_t \rho(x,t) &= \nabla \cdot (\mu \nabla \rho - \chi \rho \nabla c) \\ \Delta c &= -\rho \end{cases} \tag{6}$$

- $c(x,t)$—chemoattractant concentration
- $\rho(x,t)$—cell density, with

$$\int \rho(x,t)dx = M < \infty \text{—constant total mass} \tag{7}$$

- μ—mobility of particles, χ—chemosensitivity

[3] Independently introduced by Patlak in 1952 with applications to long-chain polymers [7].

THE SECOND MOMENT

Systems can be classified as "contracting" or "expanding" using the second moment:

$$\frac{d}{dt}\int \rho(x,t)|x|^2 dx = M\left(4\mu - \frac{\chi M}{2\pi}\right). \tag{8}$$

- Rate of change is constant, independent of initial mass distribution
- Moment can disappear in finite time, if mass is too large!

Finite time singularity formation

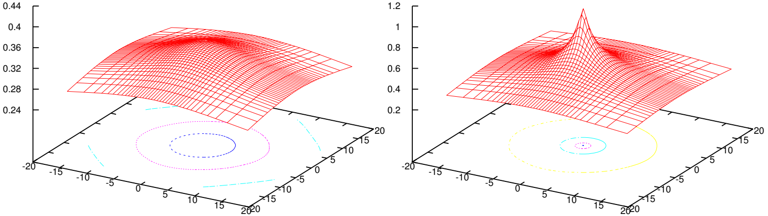


Figure: Long time snapshot of $c(x,t)$ for $M < M_c$ (left) and $M > M_c$ (right).

System (appropriately—that's the appeal!) forms a singularity in finite time if and only if it is contracting, i.e.

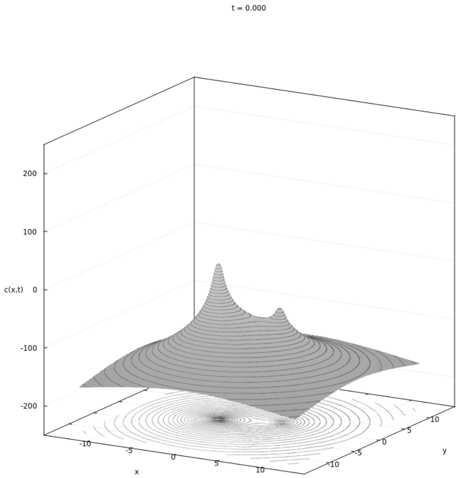
$$M > M_c = \frac{8\pi\mu}{\chi}. \tag{9}$$

Formation and interaction of singularities

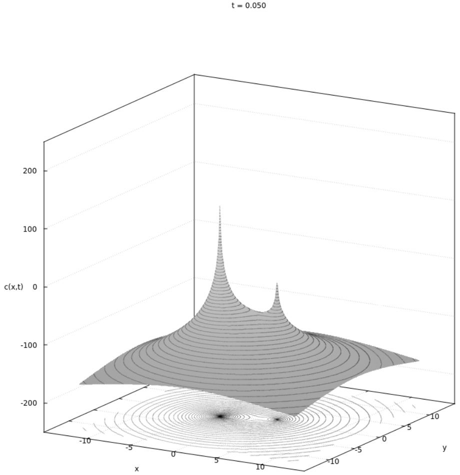
For $M > M_c$, after the formation of the first singularity [2, 8, 9]:

$$\rho(x,t) = \rho_{reg}(x,t) + \sum_{i=1}^{N_t} m_i(t)\delta\left(x - x_t^{(i)}\right). \qquad (10)$$

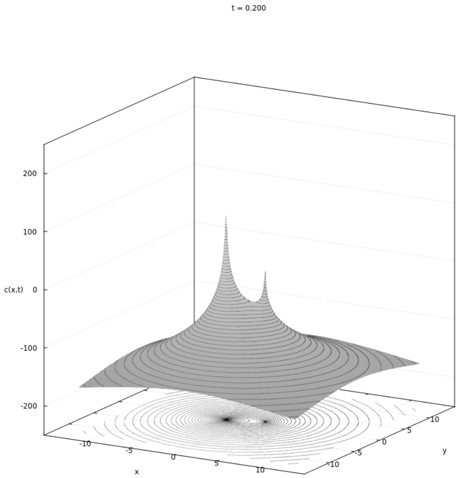
- Regular component ≈ regions of "normal" density
- Singular component ≈ K_t moving regions of very high density
- Mass is transferred from regular to singular component
- K_t increases and decreases: singularities form and merge



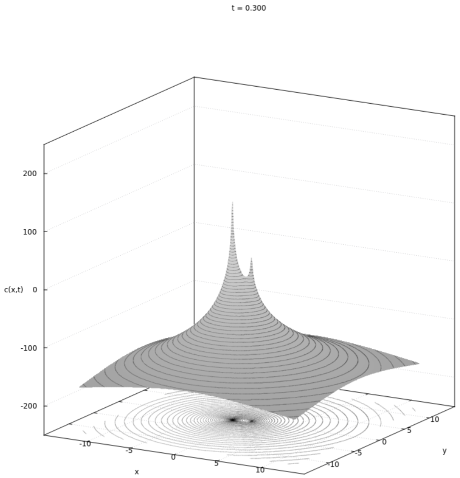
$$K_t = 0$$



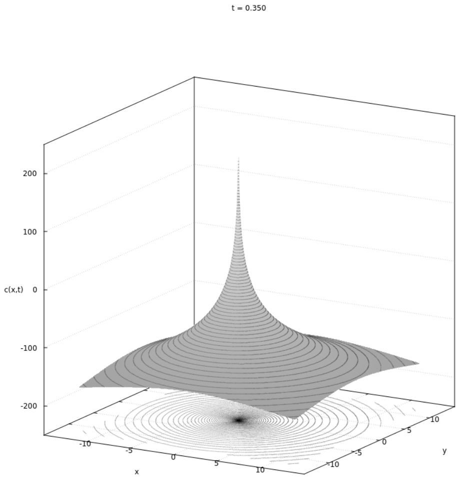
$$K_t = 2$$



$$K_t = 2$$

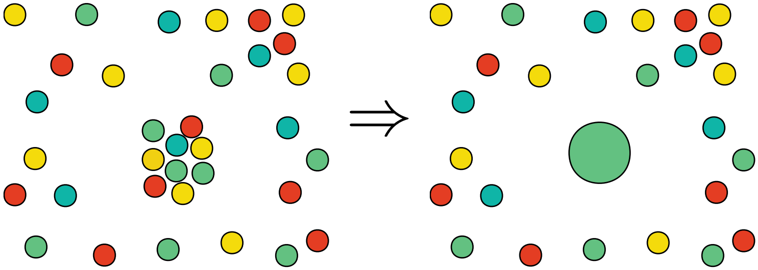


$$K_t = 2$$



$$K_t = 1$$

Coalescing



particle system

Associated particle system

- Keller-Segel:

$$\begin{cases} \partial_t \rho &= \nabla \cdot (\mu \nabla \rho - \chi \rho \nabla c) \\ \Delta c &= -\rho \end{cases} \tag{11}$$

- If c is predetermined, the first equation is a Fokker-Plank equation for

$$dX_t = \chi \nabla c(X_t, t)dt + \sqrt{2\mu} dW_t, \tag{12}$$

and so

$$P_{N_0}(x,t) = \frac{M}{N_0} \sum_n \delta\left(x - X_t^{(n)}\right) \to \rho. \tag{13}$$

- As c is unknown, we approximate it by the field generated by the N_0 particles themselves:

$$\begin{cases} dX_t^{(n)} & = \chi \nabla c_{N_0} dt + \sqrt{2\mu} dW_t^{(n)} \\ \Delta c_{N_0} & = -P_{N_0}(x,t) \end{cases} \tag{14}$$

- Since $V(x) = \frac{1}{2\pi} \ln(|x|)$ satisfies $\Delta V = \delta$, we get $c_N = -V * P_{N_0}$
- Continuous field replaced with pairwise interactions:

$$dX_t^{(n)} = -\frac{\chi}{2\pi} \sum_{1=j\neq n}^{N} \frac{M}{N_0} \frac{X_t^{(n)} - X_t^{(j)}}{\left|X_t^{(n)} - X_t^{(j)}\right|^2} dt + \sqrt{2\mu} dW_t^{(n)}. \tag{15}$$

- Particle system approximates K-S:

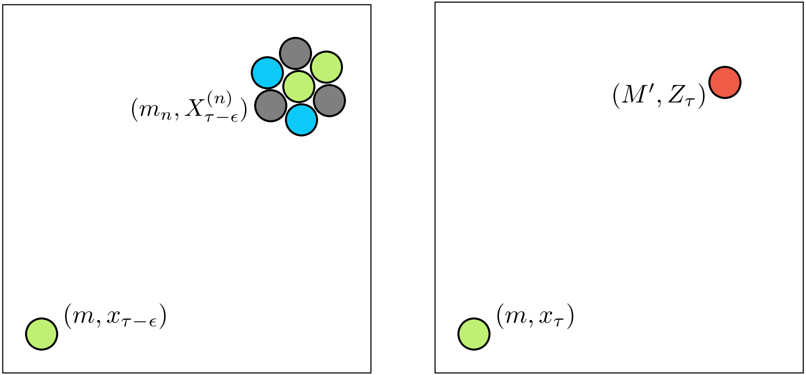
$$dX_t^{(n)} = -\frac{\chi}{2\pi} \sum_{1=j\neq n}^{N} \frac{M}{N} \frac{X_t^{(n)} - X_t^{(j)}}{\left| X_t^{(n)} - X_t^{(j)} \right|^2} dt + \sqrt{2\mu} dW_t^{(n)}. \quad (16)$$

- When K-S forms a Dirac singularity, particle system is also undefined
- This "physically" corresponds to inelastic collisions:

$$dX_t^{(n)} = -\frac{\chi}{2\pi} \sum_{1=j\neq n}^{N} m_j \frac{X_t^{(n)} - X_t^{(j)}}{\left| X_t^{(n)} - X_t^{(j)} \right|^2} dt + \sigma(m_n) dW_t^{(n)} \quad (17)$$

Diffusion coefficient

Inelastic collision:



As $\epsilon \to 0$, the drift experienced by x should coincide:

$$-\chi \sum_{i=1}^{N'} m_i \frac{\partial V}{\partial x}\left(x_{\tau-\epsilon}, X^{(i)}_{\tau-\epsilon}\right) \to -\chi M' \frac{\partial V}{\partial x}(x_\tau, Z_\tau) \Rightarrow Z_\tau = C.O.M. \tag{18}$$

Assume a general diffusion coefficient:

$$dX_t^{(n)} = -\frac{\chi}{2\pi} \sum_{i \neq n} m_i \frac{X_t^{(n)} - X_t^{(i)}}{\left| X_t^{(n)} - X_t^{(i)} \right|^2} dt + \sigma(m_n) dW_t^{(n)} \tag{19}$$

Center of mass "ghost particle" evolves similarly:

$$Z_t = \frac{1}{M'} \sum_{i=1}^{N'} m_i X_t^{(i)} \tag{20}$$

$$dZ_t = (\cdots)\, dt + \sigma(M') dW_t \tag{21}$$

By the independence of the noise, $x^2\,(\sigma(x))^2$ is linear:

$$\sigma(M') = \frac{1}{M'} \sqrt{\sum_{i=1}^{N'} m_i^2 \sigma^2(m_i)} \Rightarrow \sigma(M') = \sqrt{2\tilde{\mu}/M'} \tag{22}$$

Coalescing particle system

For N particles in $\mathbb{R}^2$:

$$dX_t^{(n)} = -\frac{\chi}{2\pi} \sum_{i \neq n} m_i \frac{X_t^{(n)} - X_t^{(i)}}{\left| X_t^{(n)} - X_t^{(i)} \right|^2} dt + \sqrt{\frac{2\tilde{\mu}}{m_n}} dW_t^{(n)} \tag{23}$$

Reduce number of particles + combine mass after inelastic collisions; heavier particles become more "deterministic"

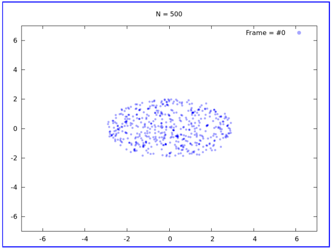
- No longer only related to K-S, because we didn't fix $\tilde{\mu}$
- Can we say anything about these collisions?

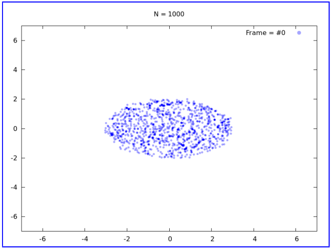
THE SECOND MOMENT

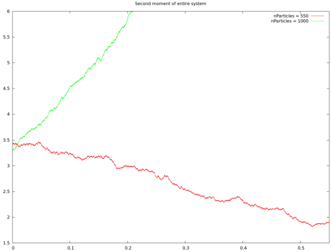
- We define the second moment process:

$$Y_t = \frac{1}{2(M)^2} \sum_{i,j=1}^{N} m_i m_j \left| X_t^{(i)} - X_t^{(j)} \right|^2 \tag{24}$$

- Characteristic squared distance between a pair of particles
- Collision $\Leftrightarrow Y_t = 0$
- Spreading out $\Leftrightarrow Y_t$ increasing


N = 500
Frame = #0
6
4
2
0
-2
-4
-6
-6 -4 -2 0 2 4 6


N = 1000
Frame = #0
6
4
2
0
-2
-4
-6
-6 -4 -2 0 2 4 6


Second moment of entire system
nParticles = 550
nParticles = 1000
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
0 0.1 0.2 0.3 0.4 0.5

Collision of full system

Some algebra gives:

$$dY_t = \left(2\tilde{\mu}\frac{2(N-1)}{M} - \frac{\chi M}{2\pi}\left(1 - \sum_j \left(\frac{m_j}{M}\right)^2\right)\right) dt + 2\sqrt{Y_t}\sqrt{\frac{2\tilde{\mu}}{M}} dW_t, \tag{25}$$

where

$$dW_t = \frac{1}{(M)^{3/2}\sqrt{Y_t}} \sum_{i,j=1}^{N} m_j \sqrt{m_i} \left(X_t^{(i)} - X_t^{(j)}\right) \cdot dW_t^{(i)}. \tag{26}$$

Classification of the origin

After rescaling:

$$dY_t = 2(\nu + 1)dt + 2\sqrt{Y_t}dW_t \tag{27}$$

$$\nu = N\left(1 - \frac{3}{2N}\right) - \frac{\chi(M)^2}{8\pi\tilde{\mu}}\left(1 - \sum_j \left(\frac{m_j}{M}\right)^2\right) \tag{28}$$

This is the squared Bessel process with index ν. We have:

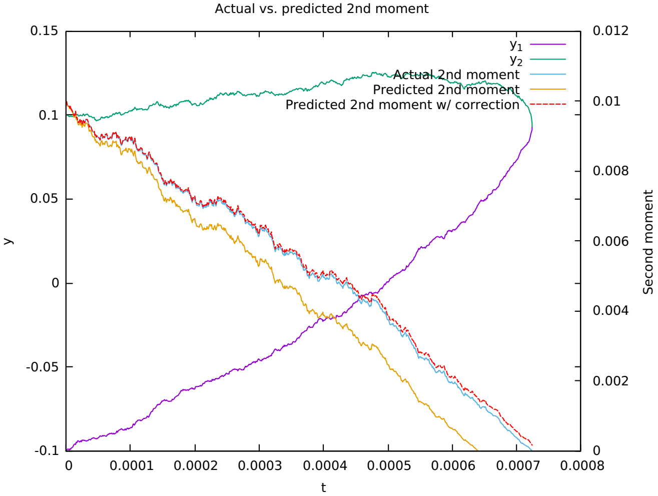
1. For $\nu \geq 0$, the origin is an entrance boundary ($Y_t > 0$ a.s. for all $t > 0$)
2. For $-1 < \nu < 0$, the origin is a regular boundary (choose behavior: absorbing, reflecting) (inelastic collision!)
3. For $\nu \leq -1$, the origin is an absorbing boundary, which is hit in finite time (inelastic collision!)

Collision of a subsystem

- Model situation: two close particles, one far one
- $\tilde{Y}_t$ is subsystem's second moment
- Ignore interactions with outside particles; then $d\tilde{Y}_t \approx dQ_t$
- With first order correction:

$$d\tilde{Y}_t \approx dQ_t - \frac{\chi m_3}{\pi} \frac{\tilde{Y}_t}{\left| X_t^{(cm)} - X_t^{(3)} \right|^2} \cos 2\theta, \tag{29}$$

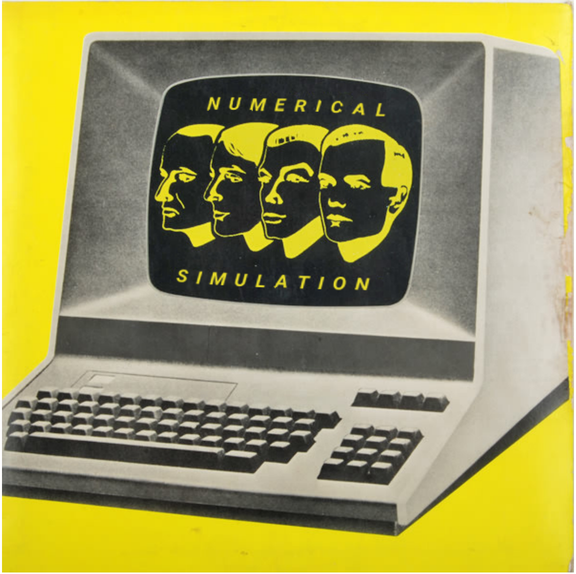
- Suggests a localized + separated subsystem becomes decoupled relative to its center of mass



An adaptive time step is used to simulate a three-particle system with $\chi = 10$, $\tilde{\mu} = 1$ and particle masses $m_1 = m_2 = 10$, $m_3 = 40$. The first two particles are initialized at $(0, \pm 0.1)$, the third at $(0, 0.4)$. The y-coordinates of the first two particles, the second moment of the subsystem, and approximations for the second moment are plotted.

Recap

- Particles carrying mass, interacting pairwise through a singular kernel
- Due to this singularity, clusters of particles may aggregate at a point
- We coalesce each aggregate into a single particle—other particles do not feel this substitution
- Particles which are about to coalesce are decoupled from the rest of the system


NUMERICAL
SIMULATION

To simulate the system, we want:

1. To avoid pairwise computations
2. To be able to detect very localized clusters which we should coalesce

Our idea:

1. Replace pairwise computations with a continuous field
2. Form an adaptive mesh at every time step to find critical, separated aggregates—then coalesce them if their second moment is predicted to vanish

Particle dynamics

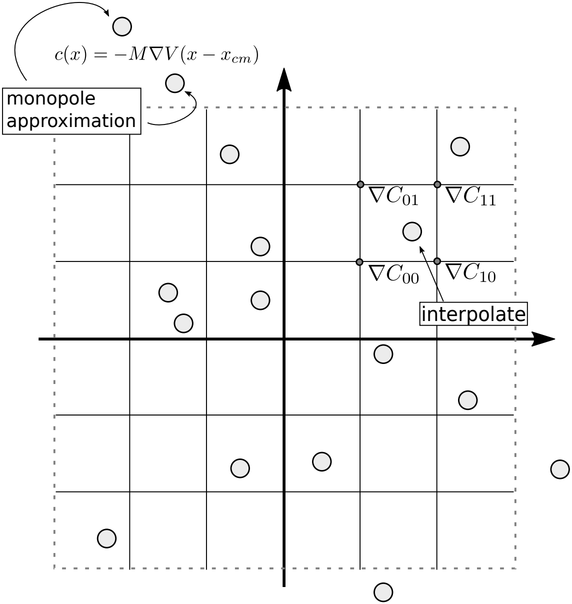
- Recall:

$$dX_t^{(n)} = -\chi \frac{\partial}{\partial X_t^{(n)}} \sum_{k \neq n} m_k V(X_t^{(n)}, X_t^{(k)}) dt + \sqrt{\frac{2\tilde{\mu}}{m_n}} dW_t^{(n)} \quad (30)$$

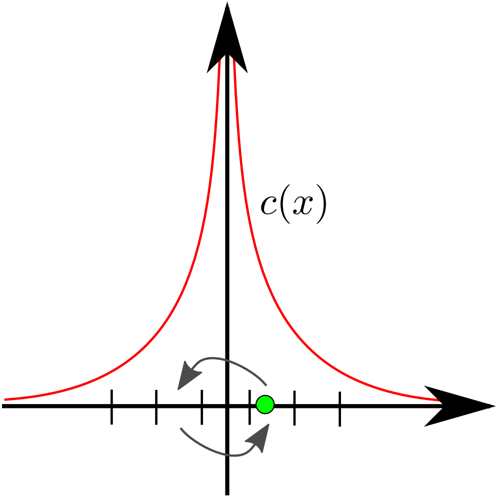
- Since $\Delta V = \delta$,

$$\begin{cases} dX_t^{(n)} & = \chi \nabla c(X_t^{(n)}, t) dt + \sqrt{\frac{2\tilde{\mu}}{m_n}} dW_t^{(n)} \\ \Delta c(x,t) & = -\sum m_i \delta\left(x - X_t^{(i)}\right) \end{cases} \quad (31)$$

- General idea:
  1. Form a grid (maybe nonlinear)
  2. Interpolate mass densities P_{ij} onto the grid points (avoids self-interaction, sticking to grid points)
  3. Solve for C_{ij}, approximate CX and CY
  4. Approximate $\nabla c(x, t)$ by interpolating CX and CY at x


$c(x) = -M\nabla V(x - x_{cm})$
monopole approximation
∇C_{01}
∇C_{11}
∇C_{00}
∇C_{10}
interpolate

Adaptive timestepping



To avoid oscillations, choose $\Delta\tau^{(i)}$ such that particle can only jump into adjacent cell $\Delta t = \Delta\tau^{(1)} + \cdots + \Delta\tau^{(k)}$

Coalescence of aggregates

General idea:

- Clustering is usually very tough, but our clusters are much simpler
- Use basic algorithm to find isolated clusters of particles, and compute the clusters' second moments
- Propagate particles through one timestep
- Use the same noise to drive the second moment process[4], and coalesce the aggregate if the moment hits zero

---

[4] For cluster-dependent α and β,

$$dY_t = \alpha dt + 2\sqrt{Y_t}\beta dW_t, \tag{32}$$

where

$$dW_t = \frac{1}{(M)^{3/2}\sqrt{Y_t}} \sum_{i,j=1}^{N} m_j \sqrt{m_i} \left(X_t^{(i)} - X_t^{(cm)} \right) \cdot dW_t^{(i)}. \tag{33}$$

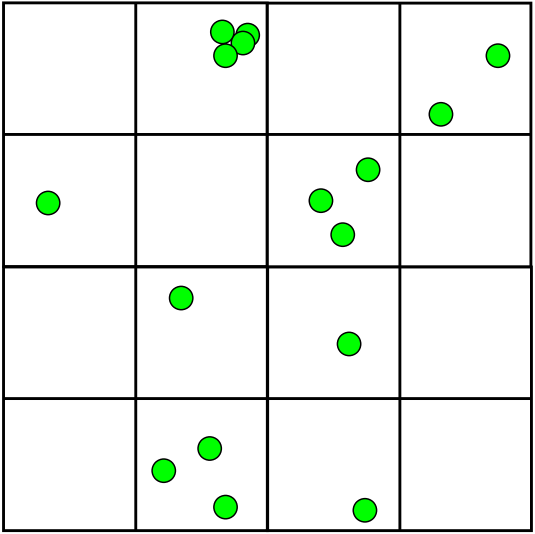
Aggregate detection

Main idea:

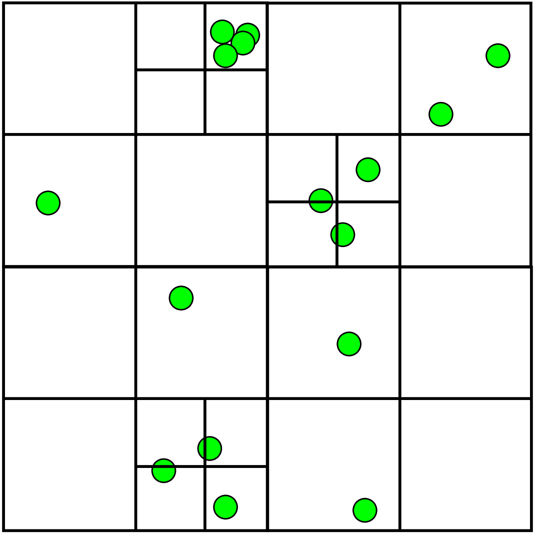
- Form an adaptive grid
- Refine cells to find aggregates which are
  1. Separated (small ratio of second moment to cell area)
  2. Likely to collide in the next time step (choose some threshold probability)
- Cells which are not separated, or are unlikely to collide in the next time step, are subdivided

Example

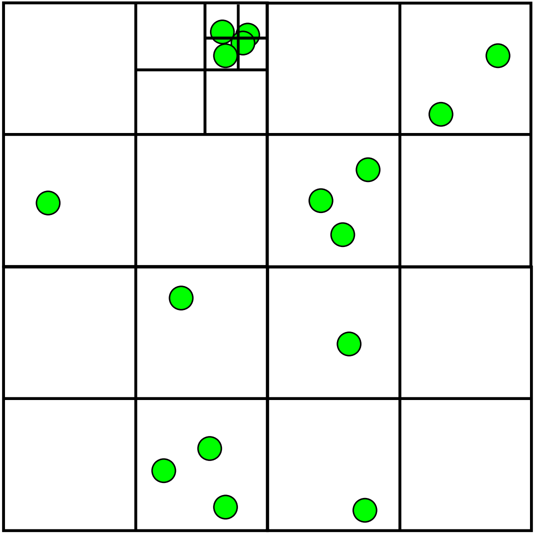
$t = 0$



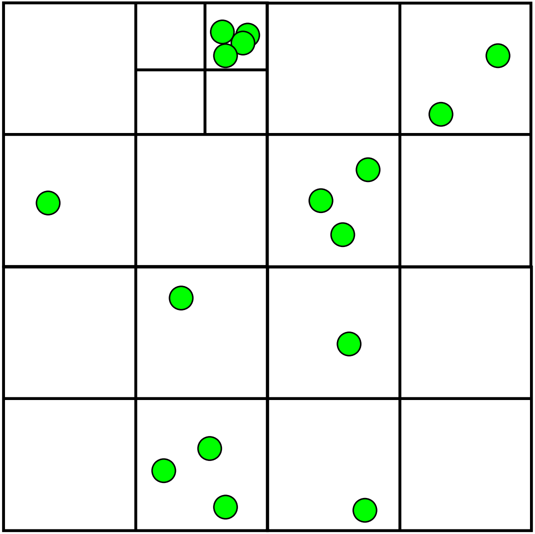
$t = 0$



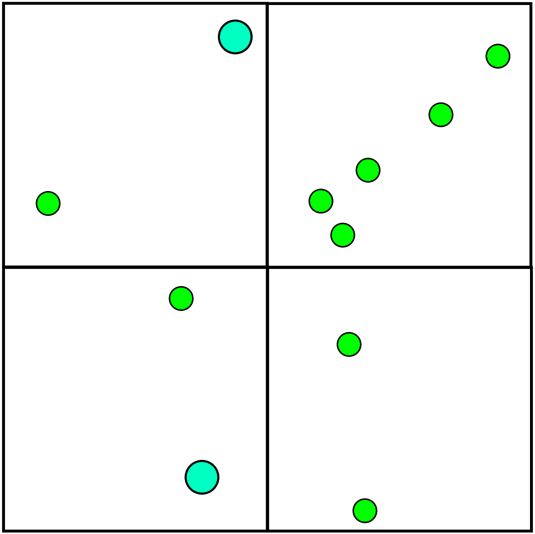
$t = 0$



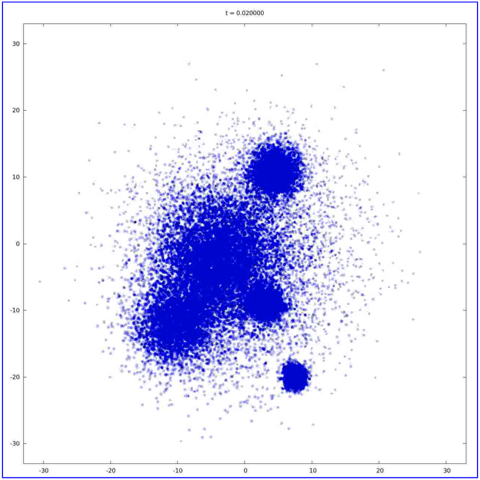
$$t = 0$$



$$t = \Delta t$$



DEFINITELY DOES SOMETHING



Note: Slightly different numerical coalescence procedure. Presented (in slides) method is more effective.

...how about something verifiable?

Nonlinear F-P equations

Keller-Segel model (again)

- Aggregation is modeled by the K-S system [5] in $\mathbb{R}^2$

$$\begin{cases} \partial_t \rho(x,t) & = \nabla \cdot (\mu \nabla \rho - \chi \rho \nabla c) \\ \Delta c & = -\rho \end{cases} \tag{34}$$

- Evolution of second moment *after blow-up*, with K_t point masses and $\bar{M}$ regular mass [2, 8, 9]:

$$\frac{d}{dt}\left(\frac{1}{M}\int |x|^2 \rho(x,t)dx\right) = 4\mu\frac{\bar{M}}{M} - \frac{\chi M}{2\pi}\left(1 - \sum_{i=1}^{K_t}\left(\frac{M_i(t)}{M}\right)^2\right). \tag{35}$$

Comparison

- Keller-Segel:

$$dX_t^{(n)} = -\frac{\chi}{2\pi}\sum_{1=j\neq n}^{N}\frac{M}{N}\frac{X_t^{(n)} - X_t^{(j)}}{\left|X_t^{(n)} - X_t^{(j)}\right|^2}dt + \sqrt{2\mu}dW_t^{(n)}. \quad (36)$$

- Our system:

$$dX_t^{(n)} = -\frac{\chi}{2\pi}\sum_{i\neq n} m_i\frac{X_t^{(n)} - X_t^{(i)}}{\left|X_t^{(n)} - X_t^{(i)}\right|^2}dt + \sqrt{\frac{2\mu}{m_n}}dW_t^{(n)} \quad (37)$$

- Small rescaling: $m_j = \frac{M}{N}$, $\mu \to \frac{\mu M}{N}$

Solving K-S and similar systems

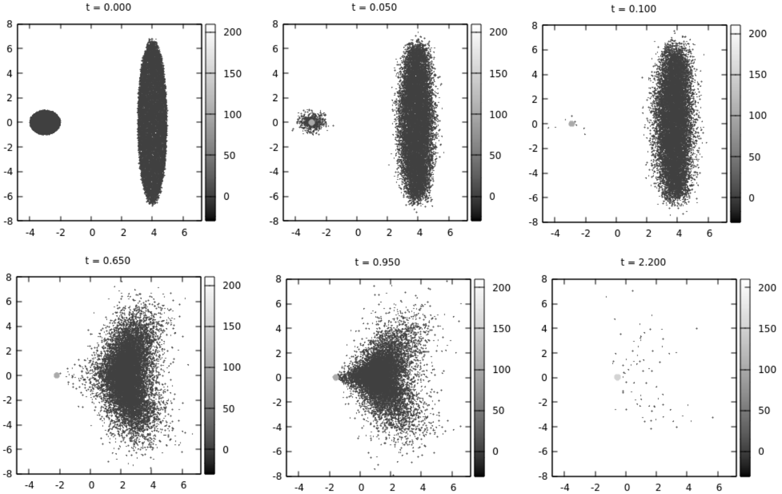
Basic idea:

- Fix large N and simulate

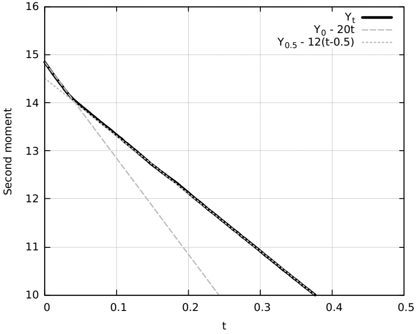
Some properties:

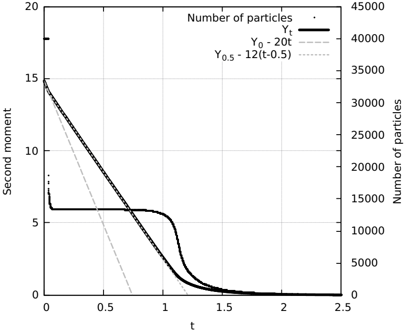
- Can simulate system post-blow-up
- Guaranteed positivity
- No spurious oscillation
- Singularities are naturally formed and evolved

CRITICAL DISC AND CLOUD

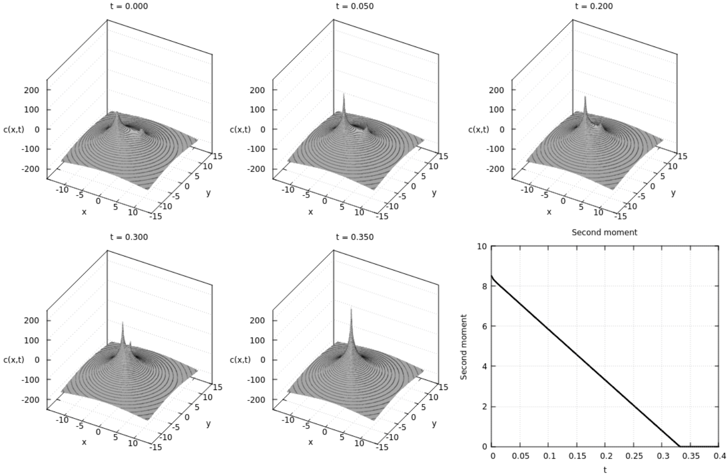


SIMULATED AND PREDICTED SECOND MOMENTS





INTERACTING SINGULARITIES



MULTISPECIES KELLER-SEGEL

- If we send $2N_0 \to \infty$ and the first N_0 particles have mass M_1/N_0 and the rest have mass M_2/N_0, we get a "two species" Keller-Segel system:

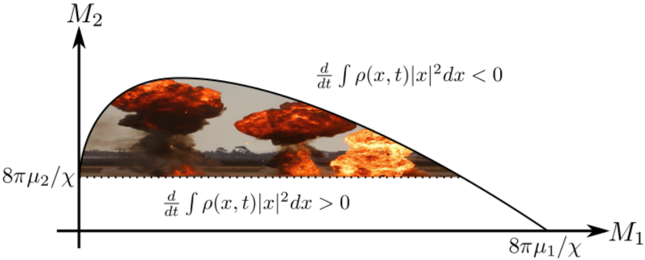
$$\begin{cases} \partial_t \rho_1 & = \nabla \cdot (\mu_1 \nabla \rho_1 - \chi \rho_1 \nabla c) \\ \partial_t \rho_2 & = \nabla \cdot (\mu_2 \nabla \rho_2 - \chi \rho_2 \nabla c) \\ \Delta c & = -(\rho_1 + \rho_1) \end{cases} \tag{38}$$

  (with maybe more than 2 components)
- Have a similar blow-up criteria for above, in terms of $\rho = \rho_1 + \rho_2$:

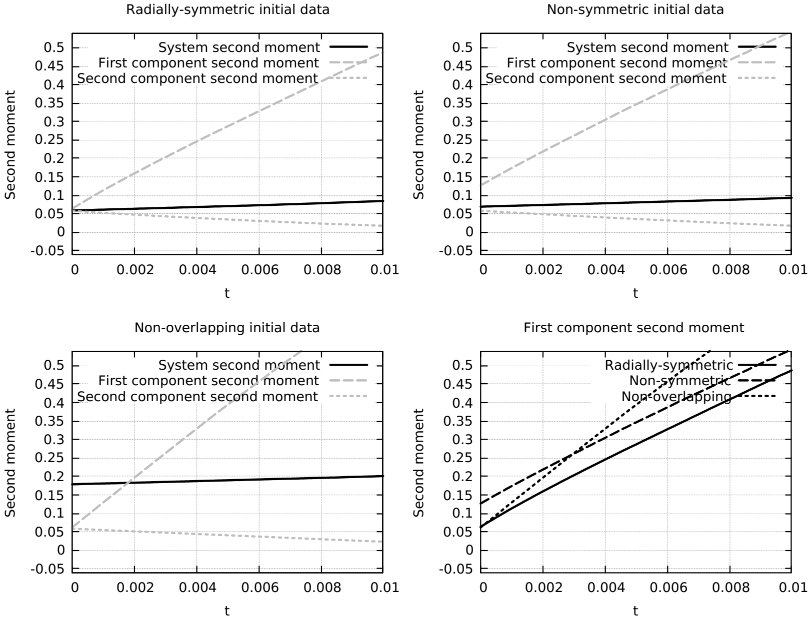
$$\frac{d}{dt} \int \rho(x,t)|x|^2 dx = \sum_\alpha \left(4\mu_\alpha - \frac{\chi M}{2\pi} \right) M_\alpha < 0 \tag{39}$$

- Is this basically just the K-S? Is the above optimal?

BLOW-UP IN THE MULTISPECIES SYSTEM



- Radial case: finite-time blow-up for an expanding system!
- Questions: Non-radial case? Which component blows up first? How do second moments evolve?
- Possibly domain-dependent behavior—finite difference can't handle the plane!
- Relevant literature: [1, 3, 4, 6]


Radially-symmetric initial data
System second moment
First component second moment
Second component second moment
Second moment
t
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
0
0.002
0.004
0.006
0.008
0.01
Non-symmetric initial data
System second moment
First component second moment
Second component second moment
Second moment
t
Non-overlapping initial data
System second moment
First component second moment
Second component second moment
Second moment
t
First component second moment
Radially-symmetric
Non-symmetric
Non-overlapping
Second moment
t

Some observations:

- System's second moment grows linearly
- Each individual component's second moment grows of decays linearly, too
- Rate appears to depend on initial distribution of mass

Other PDEs

Can apply this particle-based method to other PDEs:

$$\begin{cases} \partial_t \rho_1 & = \nabla \cdot (\mu_1 \nabla \rho_1 - \chi \rho_1 \nabla c), \\ & \vdots \\ \partial_t \rho_K & = \nabla \cdot (\mu_K \nabla \rho_K - \chi \rho_K \nabla c), \\ \mathcal{L} c & = -(\rho_1 + \cdots + \rho_K). \end{cases} \tag{40}$$

where

$$\mathcal{L} c(x,t) = \nabla \cdot (G(x) \nabla c(x,t)) + F(x,c) \tag{41}$$

Conclusion

Conclusion

Recap:

- Investigated coalescing particle system
- Developed an efficient numerical method for the simulation of the system
- Applied it to the numerical approximation and regularization of nonlinear Fokker-Planck equations

Future work:

- Add memory:

$$\partial_t c = \Delta c - k^2 c + \sum_i m_i \delta\left(x - X_t^{(i)}\right) \tag{42}$$

- Coarsening rates, etc. for non-hydrodynamic system?

Thank you for your time!

More info: https://arxiv.org/abs/1704.04873

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Effect of subsystem collision on full system

- Index change formula when subsystem collides:

$$\nu_f = \nu_i - \nu' - \frac{1}{2}, \tag{43}$$

  where ν_i and ν_f are the initial and final indices of the full system, and ν' is the index of a collided subsystem
- In the event of coalescence, restart the dynamics with less particles
- Due to this restart, the *overall* second moment might behave very differently (e.g. criticality index ν of system may flip signs)!