Asymptotic preserving schemes on kinetic models with singular limits

Changhui Tan

Department of Mathematics
Rice University

Joint work with Alina Chertock and Bokai Yan

Kinetic Descriptions of Chemical and Biological Systems:
Models, Analysis and Numerics
Iowa State University, March 23, 2017

Outline

Outline

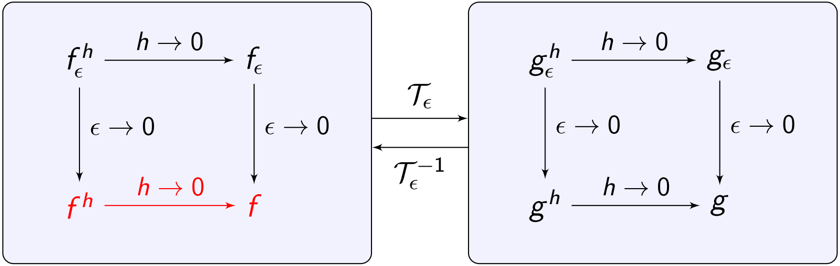
Asymptotic-preserving schemes

[Jin '99]

$$
\begin{array}{ccc}
f_\epsilon^h & \xrightarrow{h \to 0} & f_\epsilon \\
\Big\downarrow {\scriptstyle \epsilon \to 0} & & \Big\downarrow {\scriptstyle \epsilon \to 0} \\
f^h & \xrightarrow{h \to 0} & f
\end{array}
$$

- Given $f_\epsilon \to f$, design a discretization f_ϵ^h for f_ϵ that converges to the discretization f^h for f.
- *Asymptotic-preserving property*: h does not depend on ϵ.
- Extremely powerful in solving kinetic systems with hydrodynamic limits.

When the limit is singular



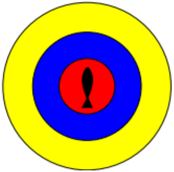
- Consider the case when f is singular, e.g. $f(t,x,v) = \rho(t,x)\delta_{v=u(t,x)}$.
- The discretization f^h can not be accurate. So f_ϵ^h is also not accurate when ϵ is small.
- **Idea:** Construct a family of invertible maps $\mathcal{T}_\epsilon$, so that $\mathcal{T}_\epsilon f_\epsilon$ converges to a non-singular profile.
- **Main Difficulty:** Find $\mathcal{T}_\epsilon$ that correctly captures the singularity.

Outline

Swarming

Three-zone models for swarms: [Reynolds '87]

- Long range: Attraction
- Short range: Repulsion
- Middle range: Alignment



- Agent-based interaction dynamics (based on Newton's second law)

$$\dot{x}_i = v_i, \quad m\dot{v}_i = F_i, \quad i = 1, \cdots, N.$$

The interaction force F_i depends on $\{x_j\}_{j=1}^N$ and $\{v_j\}_{j=1}^N$.

- Attractive/Repulsive force: $F_i(t) = -\frac{1}{N}\sum_{j\neq i} \nabla K(x_j(t) - x_i(t))$.

- Alignment force: $F_i = \frac{1}{N}\sum_{j=1}^N \phi(|x_j - x_i|)(v_j - v_i)$.

[**Cucker-Smale '07**, Motsch-Tadmor '11, Vicsek '95, ...]

Flocking [Ha-Liu '09]

Kinetic swarming models

- Vlasov-type kinetic equations

$$\partial_t f + v \cdot \nabla_x f + \frac{1}{m} \nabla_v \cdot (F(f)f) = 0,$$

where $f = f(t, x, v)$ is a probability measure in (x, v) space.

- Nonlocal interaction forces:

$$F^{CS}(f)(t,x,v) = \iint \phi(|x-y|)(v_* - v) f(t,y,v_*) dv_* dy$$
$$F^{AR}(f)(t,x,v) = \iint -\nabla_x K(x-y) f(t,y,v_*) dv_* dy.$$

- Two systems that we concern:
  1. [ARR] Attraction-Repulsion-Relaxation: $F = F^{AR} - v$.
  2. [ARA] Attraction-Repulsion-Alignment(3 zones): $F = F^{AR} + F^{CS}$

Zero inertia limit

- Consider the limit when total mass $m = \epsilon \to 0$.

$$\boxed{\partial_t f_\epsilon + v \cdot \nabla_x f_\epsilon + \frac{1}{\epsilon} \nabla_v \cdot (F(f_\epsilon) f_\epsilon) = 0,}$$

- A formal derivation of the $\epsilon \to 0$ limit ($f_\epsilon \to f$):

$$\int \nabla_v \varphi(v) \cdot F(f) f \; dv = 0.$$

$\varphi(v) = 1$: $\quad \partial_t \rho + \nabla_x \cdot (\rho u) = 0.$

$\varphi(v) = v$: $\quad$ [ARR] $u(x) = -(\nabla_x K * \rho)(x)$,

[ARA] $\int \phi(|x-y|)(u(x) - u(y))\rho(y) dy = -(\nabla_x K * \rho)(x)$.

$\varphi(v) = \frac{1}{2}|v-u|^2$: $\quad$ [ARR] $\int |v-u|^2 f(x,v) dv = 0$,

[ARA] $(\phi * \rho)(x) \int |v-u|^2 f(x,v) dv = 0$.

$$\Rightarrow \quad f(t,x,v) = \rho(t,x) \; \delta_{v=u(t,x)}.$$

Limiting system

$$f(t,x,v) = \rho(t,x)\ \delta_{v=u(t,x)}.$$

- For [ARR], the limiting system is the *aggregation equation*

$$\partial_t \rho + \nabla_x \cdot ((-\nabla_x K * \rho)\rho) = 0.$$

Wellposedness: [Laurent '07, Bertozzi-Carrillo-Laurent '09, ...]
Rigorous passage to the limit: [Jabin '99, Fetecau-Sun '15]

- For [ARA], the limiting system has an implicitly defined velocity u.

$$\partial_t \rho + \nabla_x \cdot (\rho u) = 0,$$
$$\int \phi(|x-y|)(u(x)-u(y))\rho(y)dy = -(\nabla_x K * \rho)(x).$$

Wellposedness: [Fetecau-Sun-CT '16]

Additional restriction: $\int \rho(t,x)u(t,x)dx = \int \rho_0(x)u_0(x)dx.$

Rigorous passage to the limit: [Fetecau-Sun-CT '16]

Outline

Velocity scaling: framework

$$f_\epsilon(t,x,v) \to \rho(t,x)\ \delta_{v=u(t,x)}.$$

- The transformation $\mathcal{T}_\epsilon$: rescale $f_\epsilon \leftrightarrow (g_\epsilon, u_\epsilon, \omega_\epsilon)$:

$$\boxed{f_\epsilon(t,x,v) = \frac{1}{\omega_\epsilon^d} g_\epsilon(t,x,\xi), \quad \xi = \frac{v - u_\epsilon(t,x)}{\omega_\epsilon}.}$$

- u_ϵ is the macroscopic velocity: $u_\epsilon(t,x) = \dfrac{\int v f_\epsilon(t,x,v)dv}{\int f_\epsilon(t,x,v)dv}$.
- ω_ϵ is the *scaling factor*.

Goal: choose ω_ϵ appropriately so that $g_\epsilon \to g$ and g is not singular.

Velocity scaling: history

- Kinetic system with singular equilibrium.

$$f(t,x,v) \to \rho^\infty(x)\delta_{v=v^\infty}, \quad \text{as } t \to \infty.$$

- Rescale $f \leftrightarrow (g,u,\omega)$:

$$\boxed{f(t,x,v) = \frac{1}{\omega(t,x)^d} g(t,x,\xi), \quad \xi = \frac{v-u(t,x)}{\omega}.}$$

- Linear Fokker-Planck [Filbet-Russo '04], Granular gas [Filbet-Rey '13]:

$$\omega = \sqrt{\text{Temperature}}.$$

- Kinetic flocking models [Rey-CT '16]:
  Propose a new ω and prove that $g(t,x,v) = g_0(x,v)$ for spatially "homogenous" system: $\partial_t f + \nabla_v \cdot (F^{CS}(f)f) = 0$.

Spatially "Homogenous" system

$$\partial_t f_\epsilon + \frac{1}{\epsilon}\nabla_v \cdot (F(f_\epsilon) f_\epsilon) = 0.$$

- Rewrite the system in terms of g_ϵ

$$\partial_t g_\epsilon = \left(\frac{\partial_t \omega_\epsilon}{\omega_\epsilon} + \frac{1}{\epsilon}\mathcal{A}_\epsilon\right)\nabla_\xi \cdot (\xi g_\epsilon) + \frac{1}{\omega_\epsilon}\left(\partial_t u_\epsilon - \frac{1}{\epsilon}\mathcal{B}_\epsilon\right)\cdot \nabla_\xi g_\epsilon.$$

[ARR]: $\mathcal{A}_\epsilon(t,x) = 1, \quad \mathcal{B}_\epsilon(t,x) = -u_\epsilon(t,x) - \int \nabla_x K(x-y)\rho_\epsilon(y)dy,$

[ARA]: $\mathcal{A}_\epsilon(t,x) = \int \phi(|x-y|)\rho_\epsilon(t,y)dy,$

$\mathcal{B}_\epsilon(t,x) = \int \phi(|x-y|)(u_\epsilon(t,y) - u_\epsilon(t,x))\rho_\epsilon(y)dy - \int \nabla_x K(x-y)\rho_\epsilon(y)dy.$

- It is easy to check $\partial_t u_\epsilon = \frac{1}{\epsilon}\mathcal{B}_\epsilon(t,x)$.
- Take $\omega_\epsilon(t,x) = \exp\left(-\frac{1}{\epsilon}\int_0^t \mathcal{A}_\epsilon(s,x)ds\right)$. Then $\partial_t g_\epsilon = 0$!!
  The *exact* scaling is valid for any initial configurations.

Scaling on the full system

- With free transport, the full system in terms of g_ϵ reads

$$\partial_t g_\epsilon + (u_\epsilon + \omega_\epsilon \xi) \cdot \nabla_x g_\epsilon$$
$$= \left(\frac{\partial_t \omega_\epsilon}{\omega_\epsilon} + (u_\epsilon + \omega_\epsilon \xi) \cdot \frac{\nabla_x \omega_\epsilon}{\omega_\epsilon} + \frac{1}{\epsilon} \mathcal{A}_\epsilon \right) \nabla_\xi \cdot (\xi g_\epsilon)$$
$$+ \frac{1}{\omega_\epsilon} \left(\partial_t u_\epsilon + (u_\epsilon + \omega_\epsilon \xi) \cdot \nabla_x u_\epsilon - \frac{1}{\epsilon} \mathcal{B}_\epsilon \right) \cdot \nabla_\xi g_\epsilon.$$

- Exact scaling can not be expected:
  1. The dynamics of u_ϵ:

$$\partial_t u_\epsilon + u_\epsilon \cdot \nabla_x u_\epsilon + \frac{1}{\rho_\epsilon} \nabla_x \cdot (\omega_\epsilon^2 P_\epsilon) = \frac{1}{\epsilon} \mathcal{B}_\epsilon, \quad P_\epsilon = \int \xi \otimes \xi g_\epsilon(\xi) d\xi.$$

  2. The choice of ω_ϵ:

$$\partial_t \omega_\epsilon + u_\epsilon \cdot \nabla_x \omega_\epsilon + \frac{1}{\epsilon} \mathcal{A}_\epsilon \omega_\epsilon = 0.$$

Scaling on the full system

- With free transport, the full system in terms of g_ϵ reads

$$\partial_t g_\epsilon + (u_\epsilon + \omega_\epsilon \xi) \cdot \nabla_x g_\epsilon$$
$$= (\xi \cdot \nabla_x \omega_\epsilon) \nabla_\xi \cdot (\xi g_\epsilon)$$
$$+ ((\xi \cdot \nabla_x) u_\epsilon) \cdot \nabla_\xi g_\epsilon - \frac{1}{\rho_\epsilon \omega_\epsilon} \left(\nabla_x \cdot (\omega_\epsilon^2 P_\epsilon)\right) \cdot \nabla_\xi g_\epsilon,$$

- Exact scaling can not be expected:
  1. The dynamics of u_ϵ:

$$\partial_t u_\epsilon + u_\epsilon \cdot \nabla_x u_\epsilon + \frac{1}{\rho_\epsilon} \nabla_x \cdot (\omega_\epsilon^2 P_\epsilon) = \frac{1}{\epsilon} \mathcal{B}_\epsilon, \quad P_\epsilon = \int \xi \otimes \xi g_\epsilon(\xi) d\xi.$$

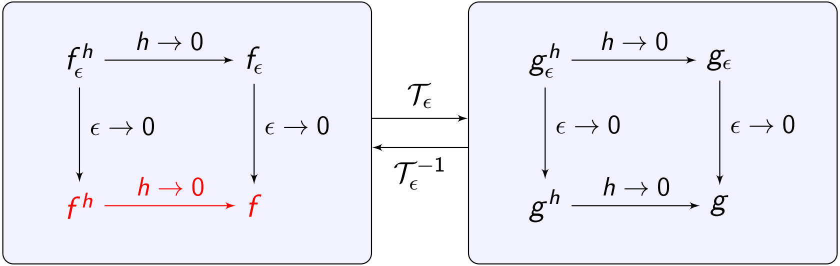
  2. The choice of ω_ϵ:

$$\partial_t \omega_\epsilon + u_\epsilon \cdot \nabla_x \omega_\epsilon + \frac{1}{\epsilon} \mathcal{A}_\epsilon \omega_\epsilon = 0.$$

Outline

Design asymptotic-preserving scheme

Recall the main idea to overcome singular limit



Two ingredients for the scheme to be asymptotic-preserving:

1. g_ϵ does not become singular as $\epsilon \to 0$.
2. An asymptotic-preserving scheme on $(g_\epsilon, u_\epsilon, \omega_\epsilon)$.

Criterion for *non-singular* $\{g_\epsilon\}$

- We call $\{g_\epsilon\}$ is non-singular if g_ϵ neither concentrate nor spread out in v, as ϵ approaches 0.

$$\max_\xi |g_\epsilon(t,x,\xi)| \le G, \quad \text{and} \quad \operatorname{supp}_\xi g_\epsilon(t,x,\xi) \subset B_R(0).$$

  for all (t,x). G, R are independent with respect to ϵ.

- Goal: Prove that under our choice of transformation $\mathcal{T}_\epsilon$, the rescaled family of solutions $\{g_\epsilon\}$ is non-singular.

Spatial oscillation

- Recall the dynamics of g_ϵ:

$$\begin{aligned}\partial_t g_\epsilon &+ (u_\epsilon + \omega_\epsilon \xi) \cdot \nabla_x g_\epsilon \\ &= (\xi \cdot \nabla_x \omega_\epsilon) \nabla_\xi \cdot (\xi g_\epsilon) \\ &+ ((\xi \cdot \nabla_x) u_\epsilon) \cdot \nabla_\xi g_\epsilon - \frac{1}{\rho_\epsilon \omega_\epsilon} \left(\nabla_x \cdot (\omega_\epsilon^2 P_\epsilon)\right) \cdot \nabla_\xi g_\epsilon,\end{aligned}$$

One major **difficulty** is to control the spacial derivatives $\nabla_x g_\epsilon, \nabla_x \omega_\epsilon, \nabla_x u_\epsilon$ and $\nabla_x P_\epsilon$ uniformly in ϵ.

- Take u_ϵ as an example. Recall its dynamics

$$\partial_t u_\epsilon + u_\epsilon \cdot \nabla_x u_\epsilon + \frac{1}{\rho_\epsilon} \nabla_x \cdot (\omega_\epsilon^2 P_\epsilon) = \frac{1}{\epsilon} \mathcal{B}_\epsilon.$$

Spatial oscillation

- One major **difficulty** is to control the spacial derivatives $\nabla_x g_\epsilon, \nabla_x \omega_\epsilon, \nabla_x u_\epsilon$ and $\nabla_x P_\epsilon$ uniformly in ϵ.
- Take u_ϵ as an example. Recall its dynamics

$$\partial_t u_\epsilon + u_\epsilon \cdot \nabla_x u_\epsilon + \frac{1}{\rho_\epsilon} \nabla_x \cdot (\omega_\epsilon^2 P_\epsilon) = \frac{1}{\epsilon} \mathcal{B}_\epsilon.$$

1. Without pressure ($P_\epsilon \equiv 0$): $\sup_{0 \le \epsilon \le \epsilon_0} \|\nabla_x u_\epsilon\|_{L^\infty} \le C$.[Tadmor-CT '14]
2. Limiting system ($u_\epsilon \to u$): $\|\nabla_x u\|_{L^\infty} \le C$.[Fetecau-Sun-CT '16]
3. Note that $u_\epsilon \to u$ weak-$\star$ in measure. Therefore, the bound on the limiting system does not imply uniform bound on $\|\nabla_x u_\epsilon\|_{L^\infty}$.

Non-oscillatory assumptions

- We assume that the solution does not have spatial oscillations:

$$
\begin{aligned}
|\nabla_x g_\epsilon(t,x,\xi)| &\le C_1 g_\epsilon(t,x,\xi), \\
|\nabla_x u_\epsilon(t,x)| &\le C_2.
\end{aligned}
$$

- The assumptions imply non-oscillatory bound for other quantities:

$$
\begin{aligned}
|\nabla_x \rho_\epsilon(t,x)| &\le C_1 \rho_\epsilon(t,x), \\
|\nabla_x P_\epsilon(t,x)| &\le C_1 P_\epsilon(t,x), \\
\|\nabla_x \omega_\epsilon(t,\cdot)\|_{L^\infty} &\le \frac{C_1(e^{C_2 t}-1)}{C_2 \epsilon} \exp\left(-\frac{c}{\epsilon} t\right).
\end{aligned}
$$

Non-oscillatory implies non-singular

Theorem ([Chertock-CT-Yan '17])

Let $(g_\epsilon, u_\epsilon, \omega_\epsilon)$ be the solution of the rescaled dynamics.
Assume the solution satisfies the non-oscillatory conditions.

Then, there exists a time $T = T(g^0) > 0$ such that $g_\epsilon(t)$ is non-singular for all $t \in [0, T]$.

- If the solution is not oscillatory in spatial variable, the proposed transformation based on velocity scaling resolves the singularity in the original limit.
- The non-oscillatory conditions can be verified numerically.

Asymptotic-preserving scheme for the rescaled system

- For $(u_\epsilon, \omega_\epsilon)$, the stiff term is *linear*. Use standard IMEX scheme.

$$\partial_t u_\epsilon + u_\epsilon \cdot \nabla_x u_\epsilon + \frac{1}{\rho_\epsilon}\nabla_x \cdot (\omega_\epsilon^2 P_\epsilon) = \frac{1}{\epsilon}\mathcal{B}_\epsilon,$$

$$\partial_t \omega_\epsilon + u_\epsilon \cdot \nabla_x \omega_\epsilon + \frac{1}{\epsilon}\mathcal{A}_\epsilon \omega_\epsilon = 0.$$

- For g_ϵ, there is no explicit dependence on ϵ. Use explicit schemes.

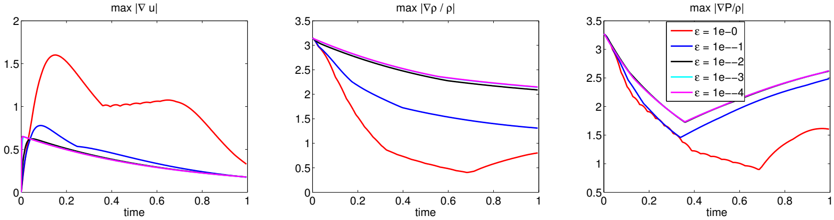
$$\partial_t g_\epsilon + \nabla_x \cdot ((u_\epsilon + \omega_\epsilon \xi) g_\epsilon) = \nabla_\xi \cdot \left[\left((\xi \cdot \nabla_x \omega_\epsilon)\xi + (\xi \cdot \nabla_x) u_\epsilon - \frac{1}{\rho_\epsilon \omega_\epsilon}\left(\nabla_x \cdot (\omega_\epsilon^2 P_\epsilon)\right)\right) g_\epsilon\right].$$

We use finite volume method, e.g. upwind.
Some corrections are introduced to ensure $\int v g_\epsilon(t, x, v) dv = 0$.
(Follow from [Rey-Tan '16])

Outline

Validation of non-oscillatory assumptions

Plots of $\max_x |\nabla_x u_\epsilon(t,x)|$, $\max_x |\nabla_x \rho_\epsilon(t,x)/\rho_\epsilon(t,x)|$ and $\max_x |\nabla_x P_\epsilon(t,x)/\rho_\epsilon(t,x)|$ for $t \in [0,1]$ and different choices of ϵ.



Initial condition:

$g^0(x,\xi) = \rho^0(x)M(\xi)$,

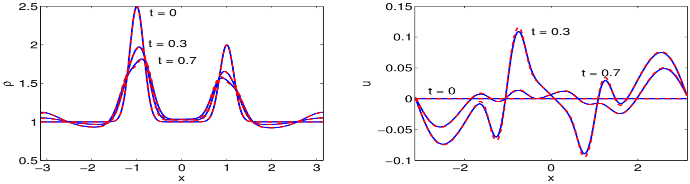
$\rho^0(x) = 1 + e^{-20(x-1)^2} + e^{-20(x+1)^2}$,

$u^0(x) = 0$,

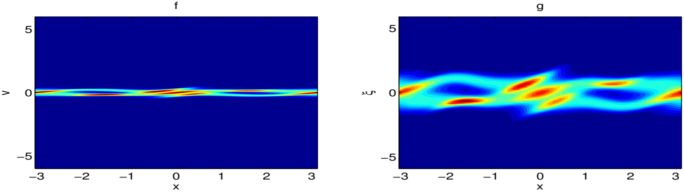
$\omega^0(x) = 1$.

Consistency test

Comparison between solving f_ϵ and $(g_\epsilon, u_\epsilon, \omega_\epsilon)$ for $\epsilon = 1$.
Snapshots of (ρ, u) at $t = 0, 0.3, 0.7$.



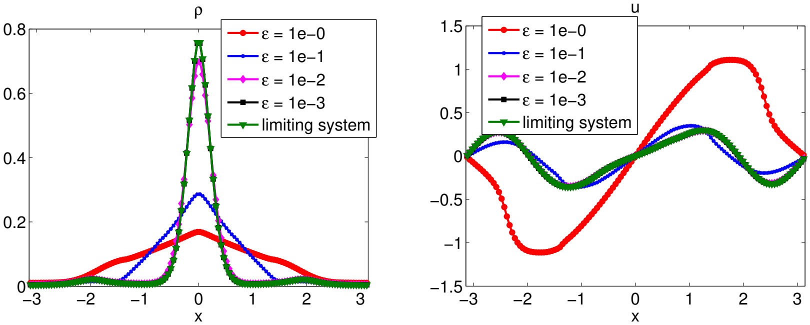
Snapshots of g at $t = 0.7$.



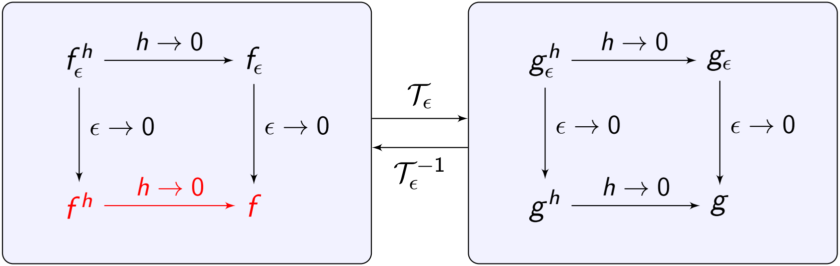
For t large or ϵ small, $f_\epsilon(t)$ is singular and the direct scheme fails.

Asymptotic-preserving test

Snapshots of $(\rho_\epsilon, u_\epsilon)$ at $t = 1$ for different ϵ. When ϵ becomes small, the profile approaches the limiting system.



Questions?



Thanks for your attention!