Numerical methods for kinetic equations of emerging collective behavior

Lorenzo Pareschi

Department of Mathematics and Computer Science
University of Ferrara, Italy

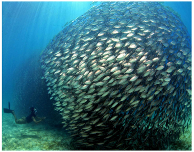
Collaborators:

G. Albi (TU Munich, Germany) **J.A. Carrillo** (Imperial College, UK)
G. Dimarco (Ferrara, Italy) **M. Herty** (Aachen, Germany)
G. Toscani (Pavia, Italy) **M. Zanella** (Ferrara, Italy)

Transport phenomena in collective dynamics: from micro to social hydrodynamics
ETH Zürich, November 1-4, 2016

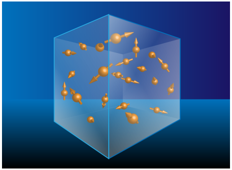
Collective behavior and self-organization

- The mathematical description of emerging collective phenomena and self-organization has gained increasing interest in various fields in *biology*, *robotics* and *control theory*, as well as *sociology* and *economics*
- Examples are groups of animals/humans with a tendency to flock or herd...


... but also interacting agents in a financial market, potential voters during political elections and connected members of a social network.


Modeling collective behavior and self-organization



Classical particles are replaced by more complex structures (*agents*, *active particles*,...). No fundamental physical laws derived from first principles and experiments cannot be reproduced.

- Various *microscopic models* have been introduced in different communities with the aim to reproduce qualitatively the dynamics and to capture some essential *stylized facts* (clusters, power laws, consensus, flocking, ...) [1]
- To analyze the formation of stylized facts and reduce the computational complexity of the agents' dynamics, it is of utmost importance to derive the corresponding *mesoscopic/kinetic* and *macroscopic dynamics* [2].

[1] *R. Hegselmann, U. Krause ('02), S. Solomon, M. Levy ('96), T. Vicsek et al. ('95), F. Cucker, S. Smale ('07); M. D'Orsogna, A. Bertozzi et al. ('06); S. Motsch, E. Tadmor ('14)*

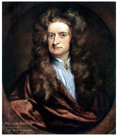
[2] *S. Cordier, L.P., G. Toscani ('05); J.A. Carrillo, M. Fornasier, G. Toscani, F. Vecil ('10); S-Y. Ha, E. Tadmor ('08); P. Degond, S. Motsch ('07); L.P., G. Albi ('12); L.P., G. Toscani ('13)*

Modeling collective behavior and self-organization

In spite of many differences between classical particle dynamics and systems of interacting agents one can apply similar methodological approaches.

microscopic models

(Newton's equations, Molecular dynamics, ...)



$\searrow$ $(N \to \infty)$

kinetic models

(Boltzmann, Enskong, Vlasov-Fokker-Planck, ...)

$\searrow$ (*equilibrium closure*)

macroscopic models

(Euler, Navier-Stokes, moment systems, ...)

Outline

1. Examples of interacting agents models
   - Opinion dynamics
   - Market economy
   - Swarming models
2. Numerical methods
   - Stochastic simulation methods
   - Asymptotically accurate entropic schemes
     - Chang-Cooper type schemes
     - Entropic average type schemes
3. Conclusions and perspectives

Examples of interacting agents models

Opinion dynamics

Evolution of N agents where each agent has an opinion $w_i = w_i(t) \in \mathcal{I}$, $\mathcal{I} = [-1, 1]$, $i = 1, \dots, N$ accordingly to an opinion averaging [3]

Averaging opinion dynamics

$$\dot{w}_i(t) = \frac{1}{N} \sum_{j=1}^{N} P(w_i, w_j)(w_j(t) - w_i(t)),$$

where $P(\cdot, \cdot) \in [-1, 1]$ characterizes the processes of *agreement/disagreement*. The corresponding binary interaction model is defined by the discrete dynamics [4]

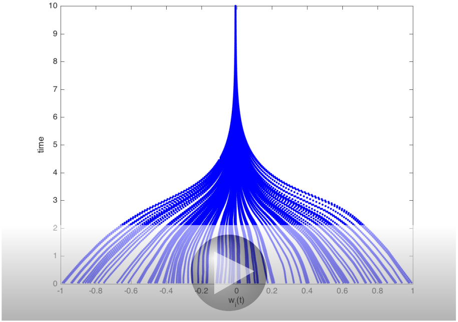
Binary opinion dynamics

$$w_i(t + \Delta t) = w_i(t)(1 - \Delta t P(w_i, w_j)) + \Delta t P(w_i, w_j) w_j(t),$$
$$w_j(t + \Delta t) = w_j(t)(1 - \Delta t P(w_j, w_i)) + \Delta t P(w_j, w_i) w_i(t).$$

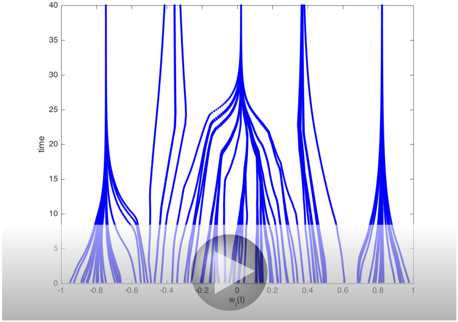
▷ An opinion dependent *noise term* modeling the *self-thinking* process and characterized by a function $D(w_i) \in [0, 1]$ may be added to the dynamics.

[3] *M.H. DeGroot ('74); R. Hegselmann, U. Krause ('02)*
[4] *G. Deffuant et al. ('00)*

Consensus



$\Delta = 0.7$, consensus is reached



$\Delta = 0.3$, opinion clusters are formed

$N = 100$ agents with *bounded confidence* model $P(w_i, w_j) = \chi(|w_i - w_j| \leq \Delta)$.

Mean-field description

The empirical measure $f_N(w,t) = \frac{1}{N}\sum_{i=1}^{N}\delta(w - w_i(t))$ as $N \to \infty$ satisfies the *mean-field* equation [5]

$$\partial_t f(w,t) + \partial_w \left(\mathcal{P}[f](w,t) f(w,t)\right) = \frac{\sigma^2}{2}\partial_w^2 (D^2(w) f(w,t)),$$

where

$$\mathcal{P}[f](w,t) = \int_{\mathcal{I}} P(w,w_*)(w_* - w) f(w_*,t)\, dw_*.$$

In some cases explicit *steady states* are known. For example if $P \equiv 1$ and $D = (1 - w^2)$ then $u = \int f w\, dw$ is conserved in time and we have

$$f_\infty(w) = \frac{C}{(1-w^2)^2}\left(\frac{1+w}{1-w}\right)^{u/(2\sigma^2)} \exp\left\{-\frac{(1-uw)}{\sigma^2(1-w^2)}\right\},$$

with C a normalization constant such that $\rho = \int f_\infty\, dw = 1$.

[5] *G. Toscani ('06); L. Boudin, F. Salvarani ('09); B. Düring, P.A. Markowich, J.F. Pietschmann, M.T. Wolfram ('09); G. Albi, L. P., G. Toscani, M. Zanella ('16)*

Boltzmann description

The binary interaction model in the limiting case $N \to \infty$ yields the following *Boltzmann equation* for $f(w,t)$ in weak form [6]

$$\partial_t \int_{\mathcal{I}} \phi(w) f(w,t)\, dw = \lambda \left\langle \int_{\mathcal{I}^2} f(w) f(w_*) \left(\phi(w') - \phi(w)\right)\, dw_*\, dw \right\rangle,$$

where

$$w' = w + \alpha P(w, w_*)(w_* - w) + \eta D(w),$$

η is a random variable with mean $\langle \eta \rangle = 0$ and variance ζ^2. In contrast with classical kinetic theory, equilibrium states of the Boltzmann model are not known.

In the *quasi-invariant limit* [7]

$$\alpha \to 0, \quad \zeta \to 0, \qquad \zeta^2/\alpha = \sigma^2, \quad \lambda = 1/\alpha$$

we recover the mean-field model (approximate equilibrium states).

[6] *G. Toscani ('06); J. Gómez-Serrano, C. Graham, J.-Y. Le Boudec ('11); G. Albi, L. P., G. Toscani, M. Zanella ('16)*

[7] *P. Degond, B. Lucquin-Desreux ('92); L. Desvillettes ('92); S. McNamara, W.R. Young ('93); C. Villani ('98)*

Market economy

Each agent has a wealth $w_i = w_i(t) \in \mathbb{R}^+$, $i = 1, \ldots, N$ which can change over a discrete time according to a generalized Lotka-Volterra dynamics [8]

Market trades dynamics

$$w_i(t+\Delta t) = w_i(t) + \frac{\Delta t}{N}\sum_{j=1}^{N} a_{ij}(w_j(t) - w_i(t)) - \frac{\Delta t}{N}\sum_{j=1}^{N} c_{ij} w_i w_j + \Delta t \eta w_i(t),$$

where $a_{ij} \in [0,1]$ characterize the *trading dynamics*, $c_{ij} \in [0,1]$ describe the competition for *limited resources* and η is a random variable with zero mean and variance σ^2 modeling the *increase/decrease of the capital* of investor i.
In a binary setting the trade becomes [9]

Binary trade dynamics

$$w_i(t+\Delta t) = w_i(t)(1 - \Delta t a_{ij} - \Delta t c_{ij} w_j(t)) + \Delta t a_{ij} w_j(t) + \Delta t \eta w_i(t),$$
$$w_j(t+\Delta t) = w_j(t)(1 - \Delta t a_{ji} - \Delta t c_{ji} w_i(t)) + \Delta t a_{ji} w_i(t) + \Delta t \eta w_j(t),$$

[8] *S. Solomon, M. Levy ('96)*
[9] *A. Chakraborti, B.K. Chakrabarti ('00)*

Mean field limit

A *mean-field* model can be derived as $N \to \infty$ and reads [10]

$$\partial_t f(w,t) + \partial_w \left((\mathcal{A}[f] - \mathcal{C}[f]w) f(w,t) \right) = \frac{\sigma^2}{2} \partial_w^2 (w^2 f(w,t)),$$

where

$$\mathcal{A}[f] = \int_{\mathbb{R}^+} a(w,w_*)(w_* - w) f(w_*)\, dw_*, \quad \mathcal{C}[f] = \int_{\mathbb{R}^+} c(w,w_*) w_* f(w_*)\, dw_*.$$

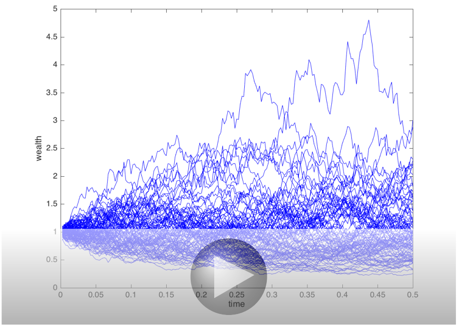
Steady states present the formation of *power-laws* and for $a \equiv 1$, $c \equiv 0$ reads

$$f_\infty(w) = \frac{(\mu-1)^\mu}{\Gamma(\mu) w^{1+\mu}} \exp\left(-\frac{\mu - 1}{w} \right)$$

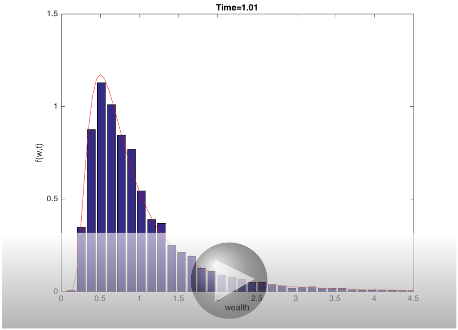
with $\mu = 1 + 2/\sigma^2 > 1$ the *Pareto exponent* and $u = \int_{\mathbb{R}} f_\infty(w) w\, dw = 1$.

[10] *J.P. Bouchard, M. Mezard ('00); S. Cordier, L. P., G. Toscani ('05); B. Düring, G. Toscani ('09)*

Emergence of power laws



$N = 100$, $\sigma = 1$



Histogram for $N = 5000$, $\sigma = 1$

Microscopic *LSS* model with $a_{ij} \equiv 1$ and $c_{ij} \equiv 0$.

Swarming models

Agents are characterized by position $x_i \in \mathbb{R}^3$, velocity $v_i \in \mathbb{R}^3$ and follow [11]

Swarming models

$$\begin{aligned}\dot{x}_i(t) &= v_i(t),\\ \dot{v}_i(t) &= \alpha v_i(t)(1-|v_i(t)|^2) + \frac{1}{N}\sum_{j=1}^{N} a(x_i,x_j)(v_j(t)-v_i(t))\end{aligned}$$

where $a(\cdot,\cdot) \in [0,1]$ defines the *alignment* and $\alpha \geq 0$ the *self-propulsion force*.

For $\alpha = 0$, the *Cucker-Smale model* corresponds to

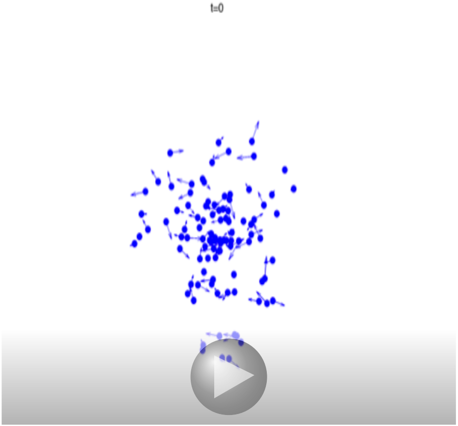
$$a(x_i,x_j) = H(|x_i - x_j|) = 1/(1+(x_i-x_j)^2)^\gamma), \qquad \gamma \geq 0.$$

If $\gamma \leq 1/2$ all agents tend to move exponentially fast with the same velocity, while their relative distances tend to remain constant (*flocking theorem*).

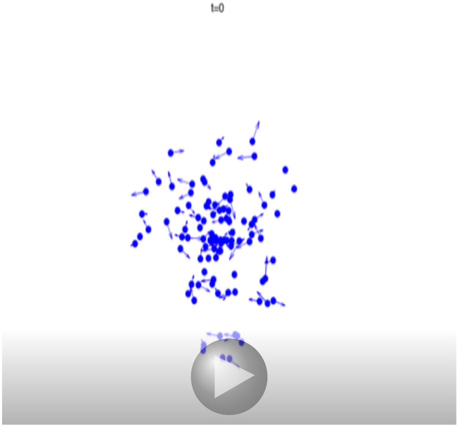
Other models considers a non symmetric alignment dynamic $a(x_i,x_j) \neq a(x_j,x_i)$, for example $a(x_i,x_j) = H(|x_i - x_j|)/\sum_k H(|x_i - x_k|)$ in *Motsch-Tadmor model*.

[11] *F. Cucker, S. Smale '07; M. D'Orsogna, A. Bertozzi et al.'06; S.Motsch, E.Tadmor ('11)*

Flocking



$\gamma = 0.25$, flocking is reached



$\gamma = 1$, no alignment

$N = 100$ agents with *Cucker-Smale* model $\alpha = 0$, $H(|x_i - x_j|) = 1/(1 + (x_i - x_j)^2)^\gamma)$

Mean-field limit

As $N \to \infty$ the empirical measure $f^N(x,v,t) = \frac{1}{N}\sum_{i=1}^N \delta(x-x_i(t))\delta(v-v_i(t))$ satisfies [12]

$$\partial_t f(x,v,t) + v\cdot\nabla_x f(x,v,t) = \nabla_v \cdot \big(\alpha v(|v|^2-1) f(x,v,t) \\ -\mathcal{H}[f](t) f(x,v,t) + D\nabla_v f(x,v,t)\big),$$

where D is a diffusion coefficient and

$$\mathcal{H}[f](t) = \int_{\mathbb{R}^3\times\mathbb{R}^3} H(|x-y|)(v_*-v) f(y,v_*,t)\, dv_*\, dy.$$

In the homogeneous case $f = f(v,t)$, exact stationary solutions can be computed

$$f_\infty(v) = C\exp\Big\{-\frac{1}{D}\Big[\alpha\frac{|v|^4}{4} + (1-\alpha)\frac{|v|^2}{2} - u_\infty v\Big]\Big\},$$

where $u_\infty = \int_{\mathbb{R}^3} v f_\infty(v)dv$.
A *phase change* phenomenon takes place as diffusion decreases [13].

[12] *S-Y. Ha, E. Tadmor ('08); A. Carrillo, M. Fornasier, G. Toscani, F. Vecil ('10)*
[13] *A.B.T. Barbaro, J.A. Cañizo, J.A. Carrillo, P. Degond '15*

Macroscopic models

- *Barbaro-Degond model:* the diffusion and social forces are simultaneously large, while the parameters of the self-propulsion are kept of order 1.
  The stationary state of the mean-field model (Gaussians) permit to close the moments equations and to obtain [14]

$$\begin{aligned} \partial_t \rho + \nabla_x \cdot (\rho u) &= 0 \\ \partial_t(\rho u) + \nabla_x \cdot (\rho u \otimes u) + D \nabla_x \rho &= -\alpha \rho u \left(|u|^2 + 5D - 1 \right). \end{aligned}$$

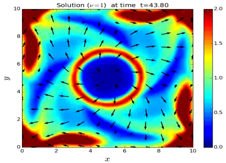
- *Ha-Tadmor model:* for $D = 0$, $\alpha = 0$, stationary states are Dirac deltas, using the mono-kinetic approximation $f(x, w, t) = \rho(x, t)\delta(v - u(x, t))$ we get [15]

$$\begin{aligned} \partial_t \rho + \nabla_x \cdot (\rho u) &= 0 \\ \partial_t(\rho u) + \nabla_x \cdot (\rho u \otimes u) &= \rho(x) \int_{\mathbb{R}^3} a(x, y) \left(u(y) - u(x) \right) \rho(y) \, dy. \end{aligned}$$

[14] *A. Barbaro, P.Degond ('12)*
[15] *S-Y. Ha, E. Tadmor ('08)*

Numerical methods

Computational considerations



The numerical solution of kinetic equations for collective behavior is challenging due to the *high dimensionality*, *preservation of structural properties* (nonnegativity, conservations) and *asymptotic steady states*.

- In particular we will focus on stochastic methods for Boltzmann equations and deterministic discretizations for mean-field problems.
- For Boltzmann-type models, we consider stochastic methods which efficiently compute the interaction integral even in the quasi invariant limit [16].
- For mean-field models, we focus on numerical schemes which preserves positivity and correctly describe the large time behavior of the system [17].

[16] *K. Nanbu ('78); G. Bird ('95); A.V. Bobylev, K. Nanbu ('00); R.E. Caflisch, L.P., G. Dimarco ('10); G. Albi, L.P. ('13); L.P., G. Toscani ('13)*

[17] *J.S. Chang, G. Cooper ('70); E.W. Larsen, D. Levermore, G.C. Pomraning, J.G. Sanderson ('85); C. Buet, S. Cordier, P. Degond, M. Lemou ('97); L. Gosse ('13); G. Albi, L.P., M. Zanella ('16)*

Prototype Boltzmann equation

The kinetic density $f = f(x, v, t)$ satisfies the Boltzmann-like equation

Boltzmann swarming

$$\partial_t f + v \cdot \nabla_x f = \lambda Q_\alpha(f, f), \quad (x, v) \in \mathbb{R}^d \times \mathbb{R}^d,$$

where the interaction term in weak form reads[18]

$$\int_{\mathbb{R}^{2d}} Q_\alpha(f, f)\phi(x, v)\, dv\, dx = \int_{\mathbb{R}^{4d}} f(x, v) f(y, w) \left(\phi(x, v') - \phi(x, v)\right)\, dw\, dy\, dv\, dx,$$

with $v' = v + \alpha H(x, y)\,(w - v)$.
In the quasi-invariant scaling, $\alpha = \varepsilon$, $\lambda = 1/\varepsilon$ we recover [19]

Mean-field swarming

$$\partial_t f + v \cdot \nabla_x f = -\nabla_v \cdot \left(\mathcal{H}[f] f\right),$$
$$\mathcal{H}[f](t) = \int_{\mathbb{R}^{2d}} H(|x - y|)(v_* - v) f(y, v_*, t)\, dv_*\, dy.$$

[18] *A.Y. Povzner ('62)*
[19] *S-Y. Ha, E. Tadmor ('08); A. Carrillo, M. Fornasier, G. Toscani, F. Vecil ('10)*

Stochastic simulation methods

- High computational cost of $Q_\alpha(f,f)$ for a product-type quadrature formula based on N parameters is $O(N^d)$.
- Structural properties (conservation of mass, momentum, ...) are difficult to preserve at the discrete level.

- Staring point is a standard *splitting method* between transport and interaction in the scaled Boltzmann equation

$$\partial_t f = -v \cdot \nabla_x f, \qquad \partial_t f = \frac{1}{\varepsilon} Q_\varepsilon(f,f).$$

- Transport step can be solved by shift of the statistical samples (free transport).
- Interaction step can be rewritten as

$$\partial_t f = \frac{1}{\varepsilon}\left[Q_\varepsilon^+(f,f) - f\right], \quad \rho = \int_{\mathbb{R}^{2d}} f\, dx\, dv = 1,$$

where $Q_\varepsilon^+ \geq 0$ is the *gain part* of the interaction operator.

An asymptotic Monte Carlo method

The *forward Euler* scheme for the interaction step writes

$$f^{n+1} = \left(1 - \frac{\Delta t}{\varepsilon}\right) f^n + \frac{\Delta t}{\varepsilon} Q_\varepsilon^+(f^n, f^n).$$

Since f^n is a probability density also $Q_\varepsilon^+(f^n, f^n)$ is a probability density. Under the restriction $\Delta t \leq \varepsilon$ then f^{n+1} is a *convex combination* of probability densities and we can construct a Monte Carlo simulation process [20].

- Taking $\Delta t = \varepsilon$, for $\Delta t \ll 1$ we approximate the mean-field model through the *asymptotic Monte Carlo algorithm* derived from [21]

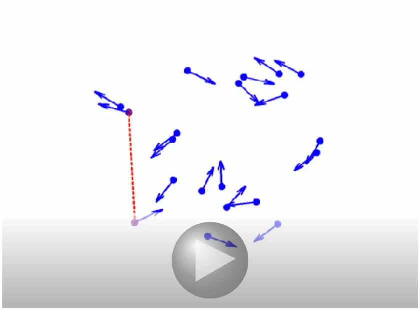
$$f^{n+1} = Q_{\Delta t}^+(f^n, f^n).$$

- The computational cost to advance one time step is *linear*, $O(N_s)$, where N_s is the number of statistical samples from f^n.
- At variance with Direct Simulation Monte Carlo (DSMC) methods, the algorithm is fully *meshless* since the binary interactions are averaged in space.

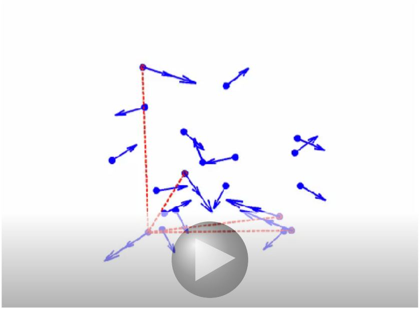
[20] *K. Nanbu ('78); G. Bird ('95)*

[21] *A.V. Bobylev, K. Nanbu ('00); R.E. Caflisch, L.P., G. Dimarco ('10); G. Albi, L.P. ('13)*

Visualization of Monte Carlo algorithms



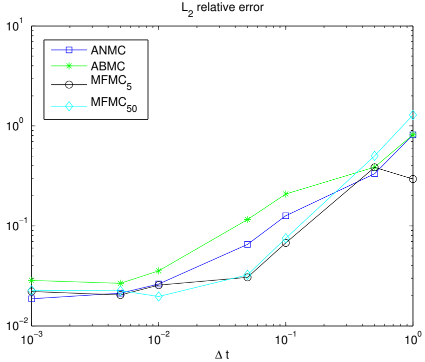
ANMC algorithm



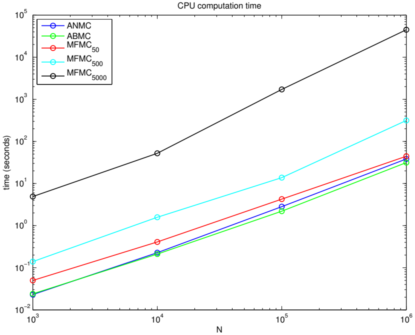
MFMC$_m$ algorithm with $m = 5$

ANMC (and ABMC) are the Boltzmann solvers based on Nanbu's and Bird's methods.
MFMC$_m$ is the random evaluation of the mean-field sum with m elements.

Accuracy and efficiency



Relative L_2 error. After $\Delta t = \varepsilon \approx \sqrt{1/N_s}$ the error is not improving, due to the statistical fluctuations.



Loglog plot of the computation times for $\Delta t = \varepsilon = 0.01$, final time is $T = 1$

Kinetic Cucker-Smale model with $N_s = 10^5$ samples.

Asymptotically accurate entropic schemes

Next we focus on the construction of numerical schemes which describe correctly the *large time behavior* of the mean-field kinetic equation [22]

Prototype Fokker-Planck equation

$$\begin{aligned}\partial_t f(w,t) &= \nabla_w \cdot \mathcal{F}[f](w,t),\\ \mathcal{F}[f](w,t) &= B[f](w,t)f(w,t) + \nabla_w (D(w)f(w,t)),\end{aligned}$$

with suitable boundary condition on w.

- Central differences typically ask for a computational grid in w which resolves the fine scales of the solution: $B[f]\Delta w \approx D(w)$.
- Upwind schemes give poor approximations of the steady state when $D(w) \neq 0$.
- In addition we require preservation of some structural properties, like nonnegativity of the solution and entropy dissipation.

[22] *J.S.Chang, G.Cooper ('70); E.W.Larsen, D.Levermore, G.C.Pomraning, J.G. Sanderson ('85); H.L. Scharfetter, H.K. Gummel ('69); C. Buet, S. Dellacherie, R. Sentis '98, C. Buet, S. Dellacherie '10, L. Gosse ('13); M. Mohammadi, A. Borzí ('15)*

Numerical flux ($d = 1$)

We introduce a uniform grid w_i, $i = 0, \dots, N$ of space Δw. We denote by $w_{i\pm 1/2} = w_i \pm \Delta w/2$ and define $f_i(t) = \frac{1}{\Delta w}\int_{w_{i+1/2}}^{w_{i-1/2}} f(w,t)\,dw$. We have

$$\partial_t f_i(t) = \frac{\mathcal{F}_{i+1/2}[f](t) - \mathcal{F}_{i-1/2}[f](t)}{\Delta w},$$

where $\mathcal{F}_{i\pm 1/2}[f](t) \approx (\mathcal{B}[f]f + D\partial_w f)(w_{i\pm 1/2})$, $\mathcal{B}[f] = B[f] + D'(w)$, is the flux function characterizing the numerical discretization.

We assume $\mathcal{F}_{i+1/2}[f]$ uses a *convex combination* of the grid values i and $i+1$

$$\mathcal{F}_{i+1/2}[f] = \tilde{\mathcal{B}}[f]_{i+1/2}\tilde{f}_{i+1/2} + D_{i+1/2}\frac{f_{i+1} - f_i}{\Delta w},$$

$$\tilde{f}_{i+1/2} = (1 - \delta_{i+1/2})f_{i+1} + \delta_{i+1/2}f_i.$$

We want to define $\delta_{i+1/2}$ and $\tilde{\mathcal{B}}[f]_{i+1/2}$ in order to satisfy *nonnegativity*, *second order accuracy*, *asymptotic preservation* and *entropy dissipation* [23].

[23] *L.P., M. Zanella ('16)*

I. Chang-Cooper type flux

Numerical flux

Imposing the numerical flux equal to zero

$$\frac{f_{i+1}}{f_i} = \frac{-\delta_{i+1/2}\tilde{\mathcal{B}}[f]_{i+1/2} + \frac{1}{\Delta w}D_{i+1/2}}{(1-\delta_{i+1/2})\tilde{\mathcal{B}}[f]_{i+1/2} + \frac{1}{\Delta w}D_{i+1/2}}.$$

By equating the ratio f_{i+1}/f_i of the numerical and the exact flux and setting

$$\tilde{\mathcal{B}}_{i+1/2}[f] = \frac{D_{i+1/2}}{\Delta w}\int_{w_i}^{w_{i+1}} \frac{1}{D(w)}\mathcal{B}[f]\,dw,$$

we recover

$$\delta_{i+1/2} = \frac{1}{\lambda_{i+1/2}} + \frac{1}{1-\exp(\lambda_{i+1/2})},$$

$$\lambda_{i+1/2} = \int_{w_i}^{w_{i+1}} \frac{1}{D(w)}\mathcal{B}[f]\,dw.$$

Exact flux

Integrating the exact stationary flux we obtain

$$\frac{f_{i+1}}{f_i} = \exp\left(-\int_{w_i}^{w_{i+1}} \frac{1}{D(w)}\mathcal{B}[f]\,dw\right).$$

In fact, from

$$\mathcal{B}[f](w,t)f(w,t) + D(w)\partial_w f(w,t) = 0,$$

in the cell $[w_i, w_{i+1}]$, we get

$$\int_{w_i}^{w_{i+1}} \left(\frac{1}{f}\partial_w f\right)(w,t)\,dw = -\int_{w_i}^{w_{i+1}} \frac{1}{D(w)}\mathcal{B}[f]\,dw.$$

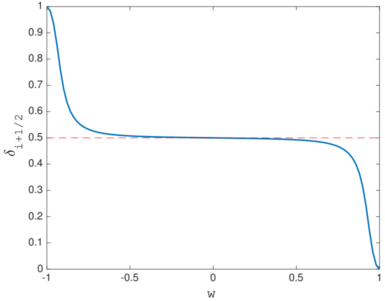
and therefore

$$\log\left(\frac{f_{i+1}}{f_i}\right) = -\int_{w_i}^{w_{i+1}} \frac{1}{D(w)}\mathcal{B}[f]\,dw.$$

▷ Note that using midpoint quadrature we have $\tilde{\mathcal{B}}_{i+1/2}[f] = \mathcal{B}[f](w_{i+1/2})$.

Remarks

- *Higher order accuracy* of the steady state can be recovered using more accurate quadrature formulas (for example open Newton-Cotes or Gaussian).
- At variance with classical Chang-Cooper discretization the weights $\delta_{i\pm 1/2}$ depend on the solution itself and therefore the scheme is *nonlinear*.
- Since $\delta_{i+1/2} \in (0,1)$ we have a convex combination of the grid values i and $i+1$ in the numerical flux



Opinion model

$w \in I = [-1,1]$

$\int_I f_0(w) w \, dw = 0$

$C(w) = (1-w^2)^2$

$B[f](w) = w + C'(w)$

$\Delta w = 0.05$

Positivity

If we consider the fully discrete explicit scheme

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} = \frac{\mathcal{F}_{i+1/2}^n - \mathcal{F}_{i-1/2}^n}{\Delta w},$$

it is easy to show the following

Proposition

Under the time step restriction

$$\Delta t \leq \frac{\Delta w^2}{2(M\Delta w + D)},$$

with $M = \max_i \left\{ |\tilde{\mathcal{B}}_{i+1/2}^n| \right\}$, $D = \max_i \left\{ D_{i+1/2} \right\}$, *we have* $f_i^{n+1} \geq 0$ *if* $f_i^n \geq 0$.

- The above result can be extended to general explicit *SSP methods* [24].
- Fully implicit schemes originate a nonlinear system of equations. However, nonnegativity holds true also in the case of *semi-implicit discretizations* where the weight functions are evaluated explicitly at time n.

[24] *S. Gottlieb, C. W. Shu, E. Tadmor '01*

Entropy for Fokker-Planck equations in bounded domains

Let us consider the equation

Fokker-Planck equation

$$\partial_t f(w,t) = \partial_w \left[(w-u) f(w,t) + \partial_w (D(w) f(w,t)) \right], \quad w \in I = [-1,1],$$

with $u = \int_I f w \, dw$ a given constant and boundary conditions

$$\partial_w (D(w) f(w,t)) + (w-u) f(w,t) = 0, \qquad w = \pm 1.$$

If we define the *relative entropy* for all positive functions $f(w,t), g(w,t)$ as follows

$$\mathcal{H}(f,g) = \int_I f(w,t) \log \left(\frac{f(w,t)}{g(w,t)} \right),$$

and denote by f^∞ the stationary state, we have [25]

$$\frac{d}{dt} \mathcal{H}(f, f^\infty) = -\mathcal{I}_D(f, f^\infty),$$

$$\mathcal{I}_D(f, f^\infty) = \int_{\mathcal{I}} D(w) f(w,t) \left(\partial_w \log \left(\frac{f(w,t)}{f^\infty(w)} \right) \right)^2 dw.$$

[25] *G. Furioli, A. Pulvirenti, E. Terraneo, G. Toscani, '16*

Numerical entropy dissipation

We can prove the following [26]

Theorem

If we define the discrete relative entropy

$$\mathcal{H}_{\Delta w}(f, f^\infty) = \Delta w \sum_{i=0}^{N} f_i \log\left(\frac{f_i}{f_i^\infty}\right)$$

for the semi-discrete Chang-Cooper type scheme we have

$$\frac{d}{dt}\mathcal{H}_\Delta(f, f^\infty) = -\mathcal{I}_\Delta(f, f^\infty),$$

where I_Δ *is the positive discrete dissipation function*

$$\mathcal{I}_\Delta(f, f^\infty) = \sum_{i=0}^{N}\left[\log\left(\frac{f_{i+1}}{f_{i+1}^\infty}\right) - \log\left(\frac{f_i}{f_i^\infty}\right)\right]\cdot\left(\frac{f_{i+1}}{f_{i+1}^\infty} - \frac{f_i}{f_i^\infty}\right)\hat{f}_{i+1/2}^\infty D_{i+1/2} \geq 0,$$

with $\hat{f}_{i+1/2}^\infty = f_{i+1}^\infty f_i^\infty \log(f_{i+1}^\infty / f_i^\infty)/(f_{i+1}^\infty - f_i^\infty) \geq 0.$

[26] *L.Pareschi, M.Zanella '16*

Free energy and gradient flow

Let us now consider the class of mean-field equations with *gradient flow structure*

Gradient flow structure

$$\partial_t f(w,t) = \nabla_w \cdot [f(w,t)\nabla_w \xi(w,t)], \qquad w \in \mathbb{R}^d$$

with no-flux boundary conditions. In case of constant diffusion $D > 0$ we have

$$\nabla_w \xi(w,t) = \mathcal{B}[f](w,t) + D\nabla_w \log f(w,t).$$

We consider the following general form for $\xi(w,t)$, $w \in \mathbb{R}^d$ [27]

$$\xi = V(w) + (U * f)(w,t) + D \log f(w,t).$$

The *free energy* associated with the model is given by

$$\mathcal{E}(t) = \int_{\mathbb{R}^d} V(w) f(w,t) dw + \frac{1}{2}\int_{\mathbb{R}^d} (U * f)(w,t) f(w,t) + D \int_{\mathbb{R}^d} f(w,t) \log f(w,t) dw$$

[27] *A.Barbaro, J.A.Cañizo, J.A.Carrillo, P.Degond '16, J.A.Carrillo, A.Chertock, Y.Huang '15*

Entropy dissipation

The dissipation of entropy along solutions is given by

$$\frac{d}{dt}\mathcal{E}(t) = -\mathcal{I}(t), \quad \mathcal{I}(t) = \int_{\mathbb{R}^d} |\nabla_w \xi|^2 f(w,t)dw.$$

The discrete version of the free energy of the system is given by

$$\mathcal{E}_{\Delta w}(t) = \Delta w \sum_{i=0}^{N} \left[\frac{1}{2} \Delta w \sum_{j=0}^{N} U_{i-j} f_i f_j + V_i f_i + D f_i \log f_i \right].$$

After time differentiation and summation by parts we obtain

$$\frac{d}{dt}\mathcal{E}_{\Delta w} = -\sum_{i=0}^{N} (\xi_{i+1} - \xi_i)\mathcal{F}_{i+1/2} = -\Delta w \sum_{i=0}^{N} \left(\tilde{\mathcal{B}}_{i+1/2} + D \log \left(\frac{f_{i+1}}{f_i} \right) \right) \mathcal{F}_{i+1/2},$$

where ξ_i is the discrete version of the potential ξ, that is

$$\xi_i = V_i + U * f_i + D \log f_i.$$

II. Entropic average flux

If we now use the Chang-Cooper type fluxes, in general, it is not possible to prove a discrete equivalent of the entropy dissipation. This can be achieved by introducing the *entropic average fluxes* defined as [28]

$$\mathcal{F}^E_{i+1/2}[f] = \tilde{\mathcal{B}}[f]_{i+1/2}\tilde{f}^E_{i+1/2} + D_{i+1/2}\frac{f_{i+1}-f_i}{\Delta w},$$
$$\tilde{f}^E_{i+1/2} = (1-\delta^E_{i+1/2})f_{i+1} + \delta^E_{i+1/2}f_i,$$

where now

$$\delta^E_{i+1/2} = \frac{f_{i+1}}{f_{i+1}-f_i} + \frac{1}{\log f_i - \log f_{i+1}} \in (0,1).$$

- The entropic average fluxes and the Chang-Cooper type fluxes define the same quantities at the steady state when $f = f^\infty$.

[28] *C. Buet, S. Dellacherie, R. Sentis '98*

Numerical entropy dissipation

Theorem

For the entropic averaged flux we have

$$\mathcal{F}^E_{i+1/2}[f] = \left(\tilde{\mathcal{B}}[f]_{i+1/2} + D_{i+1/2}\frac{\log f_{i+1} - \log f_i}{\Delta w}\right)\tilde{f}^E_{i+1/2}$$

and therefore we obtain the discrete entropy dissipation

$$\frac{d}{dt}\mathcal{E}_{\Delta w} = -\Delta w^2 \sum_{i=0}^{N}\left(\tilde{\mathcal{B}}_{i+1/2} + \frac{D}{\Delta w}\log\left(\frac{f_{i+1}}{f_i}\right)\right)^2 \tilde{f}^E_{i+1/2}.$$

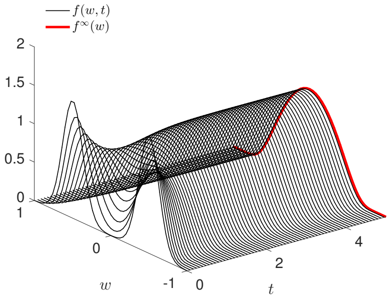
Remark: In the case of Fokker-Planck equations, like the one considered before, the entropic averaged fluxes lead to the entropy dissipation

$$\frac{d}{dt}\mathcal{H}(f, f^\infty) = -\sum_{i=0}^{N}\left[\log\left(\frac{f_{i+1}}{f^\infty_{i+1}}\right) - \log\left(\frac{f_i}{f^\infty_i}\right)\right]^2 D_{i+1/2}\tilde{f}^E_{i+1/2}.$$

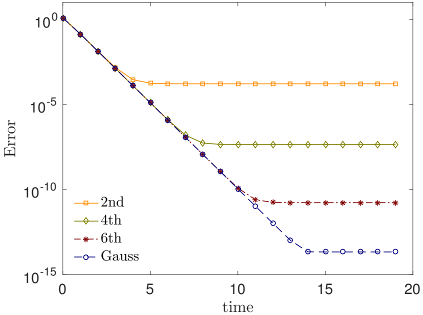
Remarks

- Nonnegativity restrictions on entropic average fluxes are *more severe* then those for Chang-Cooper type fluxes and require $D > 0$.
- Both fluxes are *second order accurate* and typically increase their order of accuracy as the solution approaches the steady state.
- In the limit case $D \to 0$ the Chang-Cooper fluxes become a standard *first order upwind* flux for the corresponding transport/aggregation problem.
- Extension to *second order upwind* fluxes in the limit $D \to 0$ are possible for Chang-Cooper type schemes.

Convergence to steady state



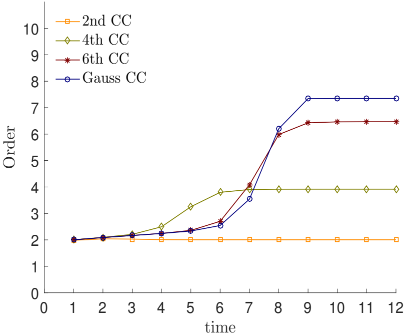
Convergence to steady state with $N = 40$



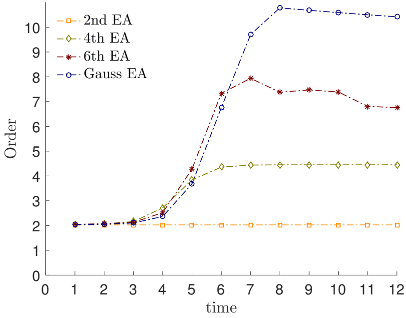
Relative error on the steady state with $N = 40$

Opinion model for $P(w, w_*) \equiv 1$, $D(w) = (\sigma^2/2)(1 - w^2)^2$ and $\sigma^2/2 = 0.1$

Accuracy test



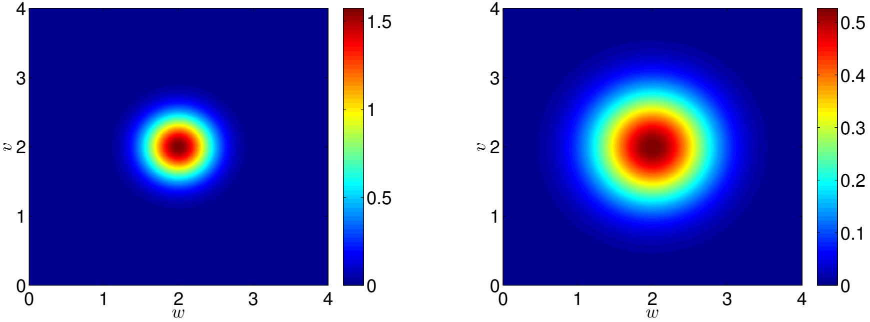
Convergence rates CC-type flux $N = 40, 80$



Convergence rates EA-type flux $N = 40, 80$

Opinion model for $P(w, w_*) \equiv 1$, $D(w) = (\sigma^2/2)(1 - w^2)^2$ and $\sigma^2/2 = 0.1$

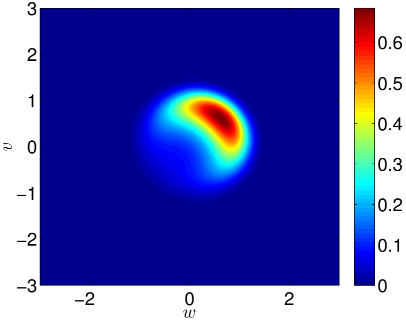
Two dimensional case



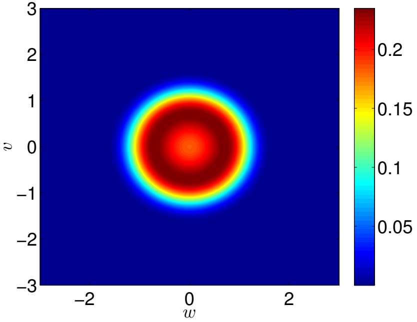
$D = 0.1$ $D = 0.3$

Swarming model for $\alpha = 0$.

Two dimensional case



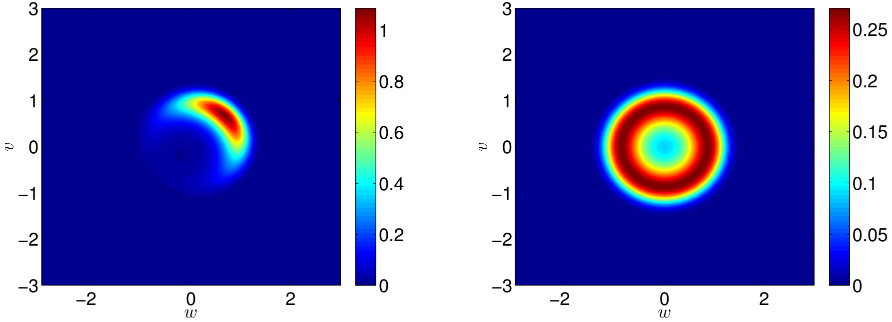
$D = 0.3$



$D = 0.5$

Swarming model for $\alpha = 2$.

Two dimensional case



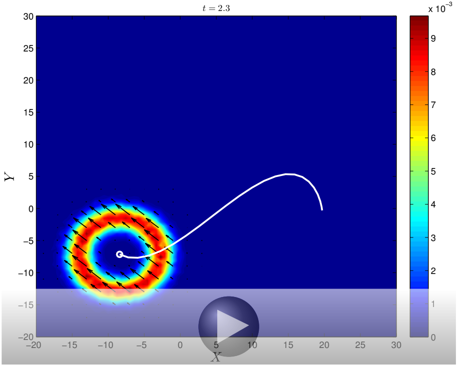
$D = 0.3$ $\quad$ $D = 0.5$

Swarming model for $\alpha = 4$.

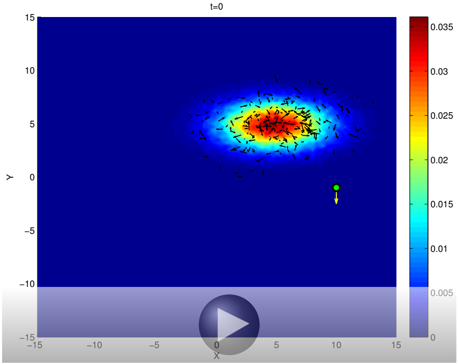
Conclusions and perspectives

- *Difficulties that distinguish the agent-based dynamics*
  - No Newtonian laws and first principles derivations
  - Active particles are not classical particles (behavioral aspects)
- *Kinetic equations can be derived for a very large number of agents*
  - Information on the large time behavior of the system
  - Development of efficient numerical tools which preserve the structural properties of the system
- *Perspectives and research directions*
  - Application of these schemes to optimal control problems where the alignment/consensus is forced by an external action or by the presence of multiple populations. For example persuading voters, influencing buyers, forcing human crowds or group of animals to follow a path.
  - Development of efficient modeling and numerical tools for the quantification of uncertainty. The introduction of stochastic parameters reflecting the uncertainty in the terms defining the interaction rules is an essential step towards more realistic applications

Mean-field control problems

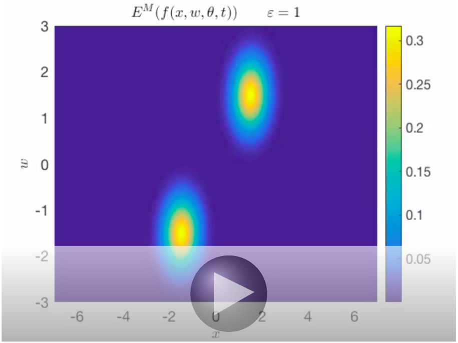


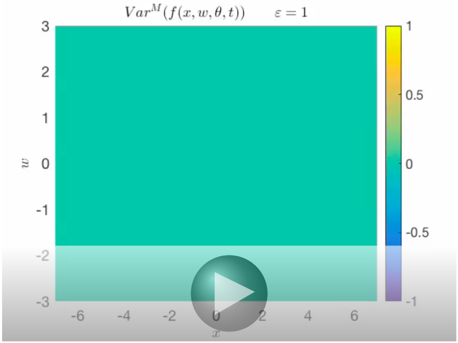
Following a desired trajectory



Following a leader

UQ in mean-field swarming





Mean-field swarming for Cucker-Smale interactions, $\alpha = 2$, $D = 0.6 + \theta/2$, $\theta \sim U([-1, 1])$.
Third order WENO in space and IMEX methods.