Uncertainty Quantification for kinetic equations of collective behavior

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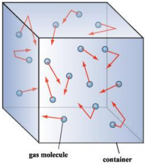
Outline

Collective behavior and self-organization

- The mathematical description of emerging collective phenomena and self–organization in systems composed of a large number of individuals has gained an increasing interest in heterogeneous research communities in biology, robotics and social sciences.




- In order reduce the computational cost of microscopic models ruling the dynamics of individual agents, it is of utmost importance to derive the corresponding kinetic and macroscopic dynamics.



The role of uncertainty

As far as the laws of mathematics refer to reality, they are not certain, and as far as they are certain, they do not refer to reality.

A. Einstein

- How can we model the realistic dynamics, since interaction forces cannot be considered as universal as the physical ones? How can we make use of the large amount of data available (from the network for example)?
- An essential step in the development of modeling real phenomena is represented by the introduction of stochastic parameters reflecting the uncertainty in the terms defining the interaction rules.[1]
- This is particularly relevant in many problems in the natural and socio-economic sciences where the interaction rules are based on observations and empirical evidence. In such cases we can have at most statistical information on the modeling parameters [2]

[1] D. Xiu '10; S. Jin, D. Xiu and X. Zhu '16; S. Jin, J. Hu '16; G. Dimarco, L. Pareschi, M.Z. '17; A. Tosin, M. Z. '18; J. A. Carrillo, L. Pareschi, M. Z. '19

[2] M. Bongini, M. Fornasier, M. Hansen, M. Maggioni '17

Uncertain kinetic modeling

Uncertain binary interactions

We consider general binary interaction models. Let us denote with $v, w \in V \subseteq \mathbb{R}$ the pre-interaction states and with $v^*, w^* \in V \subseteq \mathbb{R}$ the post-interaction states taking the general form

$$\begin{aligned} v^* &= v + \gamma \left[p_1(\theta)v + q_1(\theta)w\right] + D(v)\eta, \\ w^* &= w + \gamma \left[p_2(\theta)v + q_2(\theta)w\right] + D(w)\eta. \end{aligned}$$

where

- p_i, q_i, $i = 1, 2$ depend on random input $\theta \in I_\Theta \subseteq \mathbb{R}$, $\theta \sim \Psi(\theta)$
- $\gamma > 0$ is a given constant
- $D(\cdot)$ represents the local relevance of the diffusion
- η is a centered r.v. with finite moments (at least three).

Remark: In the introduced dynamics we considered two random quantities with radically different meanings: η represent fluctuations over the interactive part of the dynamics, thereby summarizing all sources of modification of the microscopic states that are not modelled explicitly from the binary interactions. On the other hand θ indicates a structural uncertainty in the model parameters.

Uncertain binary interactions

The aggregate behavior of the system is then described by Boltzmann-type equations for the evolution of the distribution functions $g(v,t)$, $f(\theta,v,t)$

$$\frac{d}{dt}\int_V \varphi(v) f(\theta,v,t)\,dv = \frac{1}{2}\left\langle \iint_{V^2} (\varphi(v^*)+\varphi(w^*)-\varphi(v)-\varphi(w))\, f(\theta,v,t) f(\theta,w,t)\,dv\,dw \right\rangle$$

where $\varphi(\cdot): V \to \mathbb{R}$ is a test function, and $\langle\cdot\rangle$ denotes the expectation w.r.t. η. At the numerical level we have

0. Pick $\theta \in I_\Theta$
1. Pick randomly a pair of particles: let v, w be their states
2. Update $(v,w) \to (v^*,w^*)$ with the binary rule *parametrised by* θ
3. Repeat from point 1.

A posteriori statistics of $\{f(\cdot,\cdot,\theta)\}_{\theta\in I_\Theta}$

$$\mathbb{E}[f](v,t) = \int_{I_\Theta} f(\theta,v,t)\Psi(\theta)d\theta, \qquad \mathrm{Var}(f)(v,t) = \int_{I_\Theta} f^2(\theta,v,t)\Psi(\theta)d\theta - \mathbb{E}[f]^2$$

Uncertain binary interactions

The aggregate behavior of the system is then described by Boltzmann-type equations for the evolution of the distribution functions $g(v,t)$, $f(\theta,v,t)$

$$
\begin{aligned}
&\frac{d}{dt}\int_V \varphi(v) g(v,t)\,dv \\
&\quad = \frac{1}{2}\left\langle \int_{I_\Theta}\iint_{V^2} (\varphi(v^*)+\varphi(w^*)-\varphi(v)-\varphi(w))\, g(v,t)g(w,t)\,dv\,dw d\Psi(\theta)\right\rangle \\
&\quad = Q(g,g)(v,t)
\end{aligned}
$$

where $\varphi(\cdot):V\to\mathbb{R}$ is a test function, and $\langle\cdot\rangle$ denotes the expectation w.r.t. η. At the numerical level we have

0. Pick randomly a pair of particles: let v,w be their states
1. Sample $\theta\in I_\Theta$ according to the pdf $\Psi(\theta)$.
2. Update $(v,w)\to(v^*,w^*)$ with the binary rule *parametrised by* θ
3. Repeat from point 0.

In practice we average the collision operator Q with respect to $\theta\in I_\Theta$.

Example: The Kac model

The Kac model is obtained from the introduced general binary interaction rule with the choices

$$p_1(\theta) = q_2(\theta) = \cos(\theta), \qquad p_2(\theta) = -q_1(\theta) = \sin(\theta),$$

being θ uniformly distributed in $I_\Theta = [0, 2\pi]$, i.e. $\theta \sim \mathcal{U}([0, 2\pi])$. We consider $v, w \in \mathbb{R}$ and $D \equiv 0$. The resulting Kac models have the following features

- The energy is conserved $(v^*)^2 + (w^*)^2 = v^2 + w^2$ for all $\theta \in I_\Theta$.
- The momentum is not conserved (unless $\theta = 0, 2\pi$)
- Assume $m_g(0) = \int_{\mathbb{R}} v g(v, 0) dv = 1, \qquad m_f(\theta, 0) = \int_{\mathbb{R}} v f(\theta, v, 0) dv = 1$ then $m_g(t) = e^{-t}$ and $m_f(\theta, t) = e^{(\cos(\theta)-1)t}$.
- We have $m_{\mathbb{E}[f]} = 1/2\pi \int_0^{2\pi} e^{(\cos(\theta)-1)t} d\theta$, and $m_g, m_{\mathbb{E}[f]} \to 0$ for $t \to +\infty$ but:
  - m_g goes to zero exponentially fast in time
  - $m_{\mathbb{E}[f]} \geq \dfrac{1}{\sqrt{2\pi t}} \mathrm{erf}\left(\pi \sqrt{\dfrac{t}{2}}\right) = O\left(t^{-1/2}\right)$ for $t \to +\infty$ (quite slow!)

Example: aggregation/consensus model

A basic set-up of aggregation models is derived from the general binary interaction rule

$$v^* = v + q(\theta)(w - v),$$
$$w^* = w + q(\theta)(v - w),$$

and $v, w \in \mathbb{R}$. Let us assume $q(\theta) = q_0 + \lambda\theta$ with $\theta \sim \mathcal{U}([-1,1])$, $q_0 \in (0,1)$ and $\lambda > 0$. The resulting Boltzmann models for aggregation have the following features

- The mean is conserved, indeed $v^* + w^* = v + w$. We suppose at time $t = 0$ $m_g = 0$ and $m_f = 0$.
- There is aggregation/consensus if the system converges to $\delta_0(v)$.
- We compute:
  - $E_g(t) = e^{2(q_0^2 - q_0 + \frac{1}{3}\lambda^2)t}$, for consensus $0 < \lambda < \sqrt{\dfrac{q_0(1-q_0)}{\mathrm{Var}(\theta)}}$
  - $E_f(\theta, t) = e^{2(q_0^2 - q_0 + \lambda^2\theta^2 + \lambda(2q_0 - 1)\theta)t}$
  - $E_{\mathbb{E}[f]}(t) = \dfrac{1}{4\lambda}\sqrt{\dfrac{\pi}{2t}}e^{-t/2}\left[\mathrm{erfi}(\xi_+\sqrt{t}) - \mathrm{erfi}(\xi_-\sqrt{t})\right]$, with $\xi_\pm = \pm\sqrt{2}\lambda + \frac{2q_0 - 1}{\sqrt{2}}$

Conditions for aggregation/consensus models

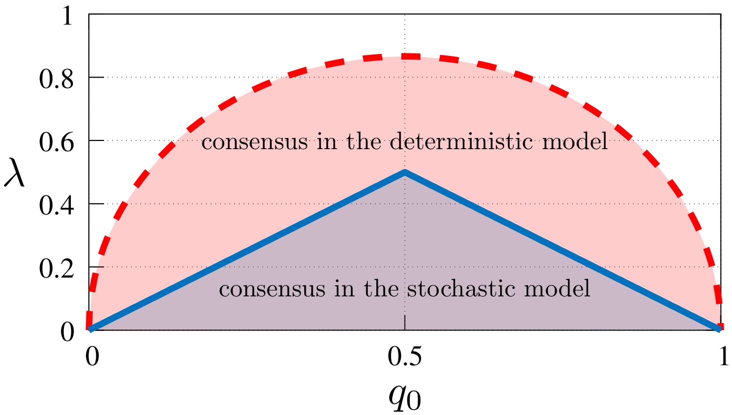
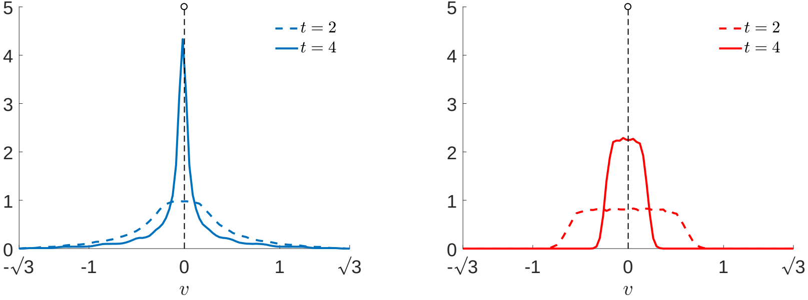


Figure: Aggregation/consensus regions in the case $\theta \sim \mathcal{U}([-1,1])$. Red: condition for the deterministic model with $\mathrm{Var}(\theta) = 1/3$. Blue: condition for the stochastic model ($0 < \lambda \leq \min\{q_0, 1-q_0\}$). We can show that $E_g = o(E_{\mathbb{E}[f]})$

Boltzmann model for aggregation/consensus



(a) $\mathbb{E}(f)(\tau, v)$ (b) $g(\tau, v)$

Figure: Approximation of transient distribution for the Boltzmann model for consensus dynamics at time steps $t = 2$, $t = 4$. The black dashed vertical line represents the asymptotic Dirac distribution centered in the (conserved) null mean. Evolution computed through standard Monte Carlo method for the Boltzmann equation (L. Pareschi, G. Russo '02; L. Pareschi, G. Toscani '13)

Fokker-Planck asymptotics

Let us concentrate to the aggregation case where the interactions read

$$v^* = v + \gamma p(\theta, v, w)(w - v) + D(v)\eta, \qquad w^* = w + \gamma p(\theta, w, v)(v - w) + D(w)\eta.$$

In order to gain a more detailed insight into the large time behavior of the introduced Boltzmann-type modeling we can resort to the so-called quasi-invariant limit. [3] In the time scale $\tau = \gamma t$ we consider

$$\gamma \to 0^+, \qquad \sigma^2/\gamma \to \sigma^2$$

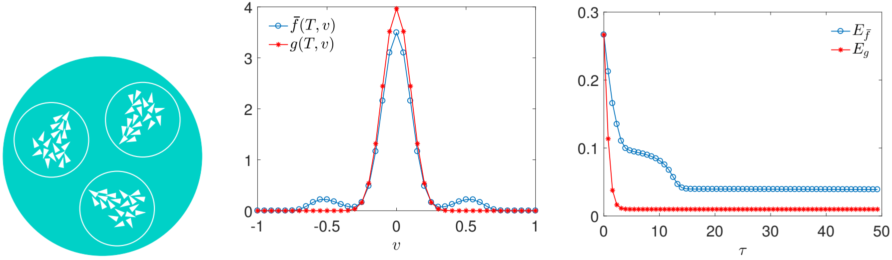
and we consider the scaled distributions $f(\theta, v, \tau/\gamma)$, $g(v, \tau/\gamma)$. Those distributions are weak solutions of the nonlocal Fokker-Planck equations

$$\partial_\tau f(\theta, v, \tau) = \nabla_v \cdot \left[\mathcal{P}[f]f + \frac{\sigma^2}{2}\nabla_v(D^2 f)\right], \qquad \mathcal{P} = \int_V P(\theta, v, w) f(\theta, v, \tau) dv$$

$$\partial_\tau g(v, \tau) = \nabla_v \cdot \left[\bar{\mathcal{P}}[g]g + \frac{\sigma^2}{2}\nabla_v(D^2 g)\right], \qquad \bar{\mathcal{P}} = \int_V \int_{I_\Theta} P(\theta, v, w) d\Psi(\theta) g(v, \tau) dv$$

[3] G. Toscani '06; C. Villani '98

Uncertain Bounded confidence case



(a) (b) (c)

Figure: (a) Sketch of bounded confidence interactions. (b) Asymptotic distributions of the deterministic and stochastic Fokker-Planck equations $v \in [-1,1]$, $D(v) = 1 - v^2$ and bounded confidence interactions $p(\theta, v, w) = \chi(|v - w| \leq \Delta(\theta))$, $\Delta(\theta) = \Delta_0 + a\theta$, $\theta \sim \mathcal{U}([-1,1])$. In particular we considered $\Delta_0 = 3/4$ and $a = 1/4$. (c) Evolution of the energies of the two models. In both cases we considered a SP method in the collocation setting. (L. Pareschi, M. Z. '18; G. Dimarco, L. Pareschi, M. Z. '17, pictures from A. Tosin, M. Z. '18)

Example: stochastic kinetic opinion model

Kinetic models for opinion formation study the evolution of a homogeneous density function $f(\theta, v, \tau)$, $v \in \mathcal{I} = [-1, 1]$ [4]

$$\partial_\tau f(\theta, v, \tau) = \partial_v \left(\mathcal{P}[f](\theta, v, \tau) f(\theta, v, \tau)\right) + \frac{\sigma^2}{2} \partial_v^2 (D(v) f(\theta, v, \tau)),$$

where

$$\mathcal{P}[f](\theta, v, \tau) = \int_{\mathcal{I}} P(v, w, \theta)(v - w) f(\theta, w, \tau)\, dw$$

is the nonlocal term. In some cases explicit steady states are known. For example if $P = P(\theta)$ and $D = (1 - v^2)^2$ then $u = \int_{\mathcal{I}} f w\, dw$ is a conserved quantity and

$$f^\infty(\theta, v) = \frac{C_{0,\theta}}{(1 - v^2)^2} \left(\frac{1 + v}{1 - v}\right)^{P(\theta)u/(2\sigma^2)} \exp\left\{-\frac{P(\theta)(1 - uv)}{\sigma^2 (1 - v^2)}\right\}$$

where $C_{0,\theta}$ is a normalization constant.

[4] G. Toscani '06; B. Düring, P.A. Markowich, J.F. Pietschmann, M.T. Wolfram '09; G. Albi, L. Pareschi, M.Z. '14; A. Tosin, M. Z. '18;

Example: stochastic kinetic wealth exchange model

The study of wealth exchanges between a large number of agents can be reduced in the following kinetic model for the evolution of the density function $f(\theta, v, \tau)$, $v \in \mathbb{R}^+$ [5]

$$\partial_\tau f(\theta, v, \tau) + \partial_v \left(\mathcal{B}[f](\theta, v, \tau) f(\theta, v, \tau)\right) = \frac{\sigma^2(\theta)}{2} \partial_v^2 (D^2(v) f(\theta, v, \tau)),$$

where

$$\mathcal{B}[f](\theta, v, \tau) = \int_{\mathbb{R}^+} \alpha(v, w)(v - w) f(\theta, w, \tau)\, dw.$$

Steady states now present the formation of power-law tails and for $\alpha \equiv 1$ and $D(v) = v$ reads

$$f^\infty(\theta, v) = \frac{(\mu(\theta) - 1)^{\mu(\theta)}}{\Gamma(\mu(\theta)) v^{1+\mu(\theta)}} \exp\left(-\frac{\mu(\theta) - 1}{v}\right), \qquad \mu(\theta) = 1 + 2/\sigma^2(\theta) > 1$$

where $\mu(\theta)$ is the so-called *Pareto exponent* and we assumed $\int_{\mathbb{R}} f^\infty(\theta, v) v\, dv = 1$.

[5] S. Cordier, L.Pareschi, G. Toscani '05; G. Furioli, A. Pulvirenti, E. Terraneo, G. Toscani '18

Example: swarming model with uncertainties

Let us consider a kinetic model for swarming with self-propulsion an diffusion [6] for the evolution of the density $f = f(\theta, x, v, \tau)$, $x \in \mathbb{R}^{d_x}$, $v \in \mathbb{R}^{d_v}$, $\theta \in \mathbb{R}^{d_\theta}$

$$\partial_\tau f(\theta, x, v, \tau) + v \cdot \nabla_x f(\theta, x, v, \tau) = \nabla_v \cdot \left[\mathcal{H}[f] f(\theta, x, v, \tau) + D(\theta) \nabla_v f(\theta, x, v, \tau))\right],$$

where now

$$\mathcal{H}[f] = \alpha(|v|^2 - 1)v + \int_{\mathbb{R}^{d_v}} \int_{\mathbb{R}^{d_x}} H(\theta, x, y)(v - w) f(\theta, y, w, \tau) dw\, dy,$$

with $\alpha > 0$ and $H(\theta; x, y) = H(\theta; |x - y|)$. In the space homogeneous case stationary solutions have the form

$$f^\infty(\theta, v) = C \exp\left\{-\frac{1}{D(\theta)}\left(\alpha \frac{|v|^4}{4} + (1-\alpha)\frac{|v|^2}{2} - u_{f^\infty}(\theta) \cdot v\right)\right\}, \qquad C > 0.$$

[6] F. Cucker, S. Smale '07; A. B. T. Barbaro, J. A. Cañizo, J. A. Carrillo, P. Degond '16

Uncertain Vlasov-Fokker-Planck modeling

All the examples of kinetic models just described are framed in the general nonlocal nonlinear Vlasov-Fokker-Planck (VFP) setting

$$
\partial_t f(\theta,x,v,t) + v\cdot\nabla_x f(\theta,x,v,t) = \nabla_v\cdot\Big[\mathcal{P}[f]f(\theta,x,v,t) + \nabla_v D f(\theta,x,v,t)\Big],
$$

where $x\in\mathbb{R}^{d_x}$, $v\in\mathbb{R}^{d_v}$ and $D\geq 0$, and we introduced the nonlocal operator

$$
\mathcal{P}[f](\theta,x,v,t) = \int_{\mathbb{R}^{d_x}}\int_{\mathbb{R}^{d_v}} P(x,y,v,w,\theta)(w-v)f(\theta,y,w,t)\,dw\,dy
$$

depending on the random input $\theta\in\mathbb{R}^{d_\theta}$, $\theta\sim\Psi(\theta)$.

Stochastic Galerkin Methods

Polynomial chaos expansions

Let us consider $v \in \mathbb{R}^d$, $d \geq 1$, the time interval $[0,T] \subset \mathbb{R}_+$ and a function

$$f(\theta, v, t) : I_\Theta \times \mathbb{R}^d \times [0,T] \to \mathbb{R}^d, \qquad f \in L^2(\Omega, \mathcal{F}, P)$$

solution of the differential problem

$$\partial_t f(\theta, v, t) = \mathcal{J}(\theta, v; f). \tag{D}$$

The *generalized polynomial chaos* method decompose the function $f(\theta, v, t)$ through a polynomial chaos expansion, i.e.

$$f(\theta, v, t) = \sum_{m \in \mathbb{N}} \hat{f}_m(v,t)\Phi_m(\theta), \tag{S}$$

where $\{\Phi_m\}_{m\in\mathbb{N}}$ is a family of polynomials defining an orthogonal basis of $L^2(\Omega, \mathcal{F}, P)$ and $\hat{f}_m$ is the *Galerkin projection* of the function f into the polynomial space

$$\hat{f}_m(v,t) = \mathbb{E}_\theta[f(\theta, v, t)\Phi_m(\theta)].$$

Polynomial chaos expansions

Truncate the series (S) up to order M and obtain

$$f^M = \sum_{m=0}^{M} \hat{f}_m(v,t)\Phi_m(\theta)$$

and consider the Galerkin projections of the differential problem (D)

$$\partial_t \mathbb{E}_\theta[f(\theta,v,t)\Phi_\Psi(\theta)] = \mathbb{E}_\theta\left[\mathcal{J}(\theta,v;f^M)\Phi_\Psi(\theta)\right], \qquad h=0,\dots,M.$$

In general we have obtained a coupled system of $M+1$ deterministic equations

$$\partial_t \hat{f}_h(v,t) = \mathcal{J}(v,(\hat{f}_k)_{k=0}^M), \qquad h=0,\dots,M$$

whose solution spectrally converges to the solution of the original problem (D) under suitable conditions.
Statistical quantities of interest are defined in terms of the projections:

$$\mathbb{E}_\theta[f(\theta,v,t)] \approx \hat{f}_0(v,t), \qquad \mathrm{Var}(f(\theta,v,t)) \approx \sum_{h=0}^{M} \hat{f}_h^2(v,t)\mathbb{E}_\theta[\Phi_h^2(\theta)] - \hat{f}_0^2(v,t)$$

Polynomial chaos expansion for mean-field problems

Let us consider the initial nonlinear VFP problem with nonlocal drift

$$\mathcal{P}[f](\theta,x,v,t) = \int_{\mathbb{R}^{d_x}}\int_{\mathbb{R}^{d_v}} P(x,y,v,w,\theta)(v-w)f(\theta,y,w,t)dw\,dy.$$

The gPC-SG formulation of the mean–field equation is given by the following system of deterministic differential equations $h = 0,\dots,M$

$$\begin{aligned}\partial_t \hat{f}_h(x,v,t) + v\cdot\nabla_x \hat{f}_h(x,v,t) &= \\ \nabla_v \cdot \Big[\sum_{k=0}^{M} P_{hk}[\hat{f}](x,v,t)\hat{f}_k(x,v,t) + \nabla_v D(v)\hat{f}_h(x,v,t)\Big],\end{aligned}$$

where

$$P_{hk}[\hat{f}](x,v,t) = \frac{1}{\|\Phi_h^2\|}\sum_{m=0}^{M}\int_{I_\Theta}\mathcal{P}[\hat{f}_m]\Phi_k(\theta)\Phi_m(\theta)\Phi_\Psi(\theta)d\Psi(\theta).$$

Stability of the gPC decomposition

We indicate with $\|\hat{\mathbf{f}}\|_{L^2}$ the standard L^2 norm of the vector $\hat{\mathbf{f}} = (\hat{f}_0, \dots, \hat{f}_M)$. We can easily observe that $\|f^M\|_{L^2(\Omega)} = \|\hat{\mathbf{f}}\|_{L^2}$ thanks to the orthogonality of $\{\Phi_k(\theta)\}_{k=0}^M$ in $L^2(\Omega)$

$$\|f^M\|_{L^2(\Omega)} = \int_{I_\Theta} \int_{\mathbb{R}^{d_x} \times \mathbb{R}^{d_v}} \left(\sum_{k=0}^M \hat{f}_k \Phi_k(\theta) \right)^2 dv dx d\Psi(\theta)$$

and we have[7]

Theorem

If $\|\nabla_v P_{hk}\|_{L^\infty} \leq C$, with $C > 0$ for all $h, k = 0, \dots, M$ then we have

$$\|\hat{\mathbf{f}}\|^2_{L^2} \leq e^{t(C+2)} \|\hat{\mathbf{f}}(0)\|^2_{L^2}$$

[7] J. A. Carrillo, M. Z. in progress

Problems and challenges

In vector notations to introduced problem reads

$$\partial_t \hat{\mathbf{f}}(x,v,t) + v \cdot \nabla_x \hat{\mathbf{f}}(x,v,t) = \nabla_v \cdot \Big[\mathbf{P}[\hat{\mathbf{f}}](x,v,t)\hat{\mathbf{f}}(x,v,t) + \nabla_v \mathbf{D}(v)\hat{\mathbf{f}}(x,v,t) \Big],$$

where $\hat{\mathbf{f}} = (\hat{f}_0, \dots, \hat{f}_M)^T$, $\mathbf{P} = (P_{hk})_{h,k=0}^M$ and $\mathbf{D}$ is a diagonal matrix. In the introduced problem uncertainty increases the dimensionality and the complexity of the kinetic modelling [8]. Hence, the development of numerical methods presents several difficulties due to the intrinsic structural properties of the solution

- Non negativity of the distribution function
- Conservation of invariant quantities
- Entropy dissipation
- Accurate description of the steady states

[8] G. Dimarco, L. Pareschi, M. Z. '17; J. A. Carrillo, L. Pareschi, M. Z. '18

gPC–SP schemes for simplified mean-field problems

Let us consider first the case in which the uncertainty comes only from the initial data and $\mathcal{P}[f](x,v,t) = P(x,v,t)$ is independent of f. Then the matrix **P** is diagonal and we need to solve the decoupled set of equations

$$\partial_\tau \hat{f}_h(x,v,t) + v \cdot \nabla_x \hat{f}_h(x,v,t) = \nabla_v \cdot [P_{hh}(x,v,t)\hat{f}_h(x,v,t) + \nabla_v D(v)\hat{f}_h(x,v,t)], \qquad h = 0,\dots,M$$

A structure preserving scheme [9] can be implemented for each $\hat{f}_h(x,v,t)$ to preserve the asymptotic behavior of each gPC projection (and its positivity).
Remark: For a more general $\mathcal{P}$, however, the SP approach cannot be applied and the construction of a gPC expansion which preserves the steady state is challenging.

[9] L. Pareschi, M. Z. '18

Micro–Macro decompositions

Let us concentrate on the homogeneous setting in $d_v = 1$ to simplify notations. We obtain the nonlinear nonlocal Fokker-Planck problem with uncertainties

$$\partial_t f(\theta, v, t) = \mathcal{J}(f, f)(\theta, v, t)$$

where

$$\mathcal{J}(f, f)(\theta, v, t) = \partial_v \Big(\mathcal{P}[f](\theta, v, t) f(\theta, v, t) + \partial_v D(v) f(\theta, v, t) \Big),$$

and assume it admits the unique steady state f^∞. We consider the micro-macro decomposition

$$f = f^\infty + g,$$

where $g = g(\theta, v, t)$ is s.t. $\int g\phi(v)\, dv = 0$ for some moments (ex. $\phi(v) = 1, v$). Since it is easily seen that $\mathcal{J}(f^\infty, f^\infty) = 0$ we obtain

$$\mathcal{J}(f, f) = \mathcal{J}(g, g) + \mathcal{L}(f^\infty, g), \qquad \mathcal{L}(f^\infty, g) = \partial_w \Big(\mathcal{P}[f^\infty] g + \mathcal{P}[g] f^\infty \Big).$$

Note that, the only admissible steady state is now $g \equiv 0$.

Micro–Macro gPC approximation

We consider now the gPC approximation as

$$\begin{cases} \partial_t \hat{g}_h(v,t) = \hat{\mathcal{J}}_h(\hat{g},\hat{g}) + \hat{\mathcal{L}}_h(\hat{f}^\infty,\hat{g}), \\ f^M = f^{\infty,M} + g^M, \end{cases}$$

where

$$\hat{\mathcal{J}}_h(\hat{g},\hat{g}) = \partial_v \left[\sum_{k=0}^{M} P_{hk}[\hat{g}]\hat{g}_k(v,t) + \partial_v D(v)\hat{g}_k(v,t) \right],$$

$$\hat{\mathcal{L}}_h(\hat{f}^\infty,\hat{g}) = \partial_v \left[\sum_{k=0}^{M} \left(P_{hk}[\hat{f}^\infty]\hat{g}_k(v,t) + P_{hk}[\hat{g}]\hat{f}_k^\infty(v,t) \right) \right].$$

Proposition

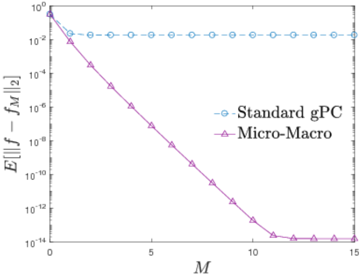
The function $g^M = 0$ is an admissible local equilibrium of the micro-macro gPC scheme and therefore $f^M = f^{\infty,M}$ is a local equilibrium state.

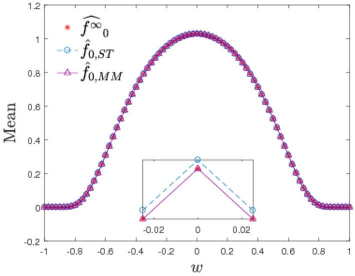
Micro–Macro gPC: Opinion dynamics

The stationary solution of the opinion model with $P(\theta) = 0.5 + 0.25\theta$, $\theta \sim \mathcal{U}([-1,1])$ and $D(v) = \frac{\sigma^2}{2}(1-v^2)^2$ is given by

$$f^\infty(v;\theta) = \frac{C}{(1-v^2)^2}\left(\frac{1+v}{1-v}\right)^{P(\theta)u/(2\sigma^2)} \exp\left\{-P(\theta)\frac{(1-uv)}{\sigma^2(1-v^2)}\right\}.$$

We consider central difference discretizations of the derivatives in w and compare a standard gPC approximation with the micro-macro gPC approximation (residual equilibrium scheme).





Opinion dynamics Bounded Confidence case [10]

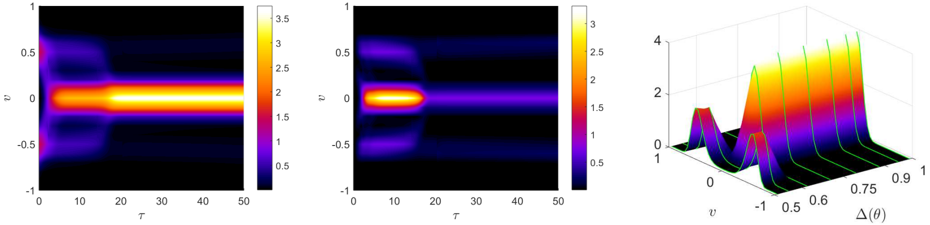


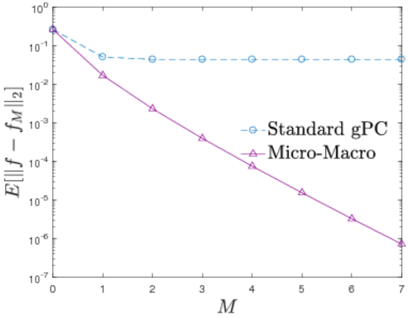
Figure: Evolution of the bounded confidence model with $P(\theta, v, w) = \chi(|v - w| \leq \Delta(\theta))$, $\Delta(\theta) = 3/4 + 1/4\theta$, $\theta \sim \mathcal{U}([-1, 1])$, $v, w \in [-1, 1]$. Left: $\mathbb{E}_\theta[f]$. Right: $\mathrm{Var}(f)$. Time interval $t \in [0, 50]$.

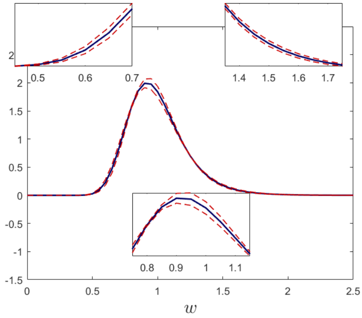
[10] R. Hegselmann, U. Krause '02; A. Tosin, M. Z. '18

Micro–Macro gPC: Wealth evolution

The stationary solution for the mean–field wealth model can be obtained for $a(w, w_*) \equiv 1$ and $D(v,\theta) = \frac{\sigma^2(\theta)}{2} v^2$, with $\theta \sim \mathcal{U}([-1,1])$

$$f^\infty(v;\theta) = \frac{(\mu-1)^\mu}{\Gamma(\mu) v^{1+\mu}} \exp\left\{ -\frac{\mu-1}{v} \right\}, \quad \mu(\theta) = 1 + 2/\sigma^2(\theta), \quad \sigma^2 = 0.1 + 0.05\theta$$





Micro-Macro gPC: swarming with phase transition

Micro-Macro gPC: 2D swarming with phase transition

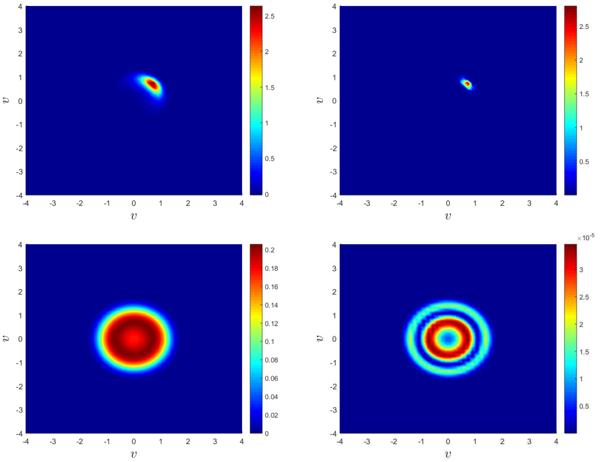
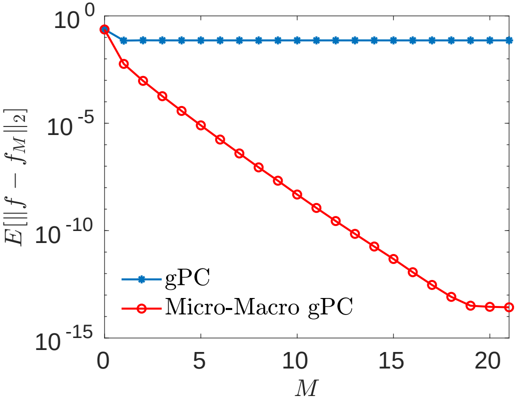


Figure: Top row: 2D swarming model with $D(\theta) = 0.15 + 0.1\theta$, large time left mean distribution right variance. Bottom row: 2D swarming model with $D(\theta) = 0.75 + 0.1\theta$, large time left mean distribution right variance.

Micro-Macro gPC: swarming with phase transition



Monte Carlo gPC Methods

Microscopic version

In absence of diffusion all the introduced kinetic models can be derived from a second order system of ODEs for $(x_i(\theta,t), v_i(\theta,t)) \in \mathbb{R}^{d_x} \times \mathbb{R}^{d_v}$, $i = 1,\dots,N$ with the general structure [11]

$$\begin{cases} \dot{x}_i(\theta,t) &= v_i(\theta,t), \\ \dot{v}_i(\theta,t) &= S(\theta; v_i) + \dfrac{1}{N}\displaystyle\sum_{j=1}^{N} [H(\theta; |x_i - x_j|)(v_j - v_i) + \\ & \qquad A(\theta, x_i, x_j) + R(\theta, x_i, x_j)] \end{cases}$$

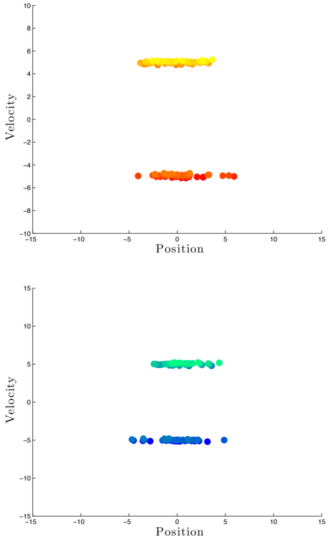
where $S(\theta, v_i)$ is a self-propelling term, $H(\theta, |x_i - x_j|)$ the alignment process, $A(\theta, x_i, x_j)$ the attraction dynamics and $R(\theta, x_i x_{,j})$ the short-range repulsion.

Proposition

In the pure alignment case with $H = K(\theta)/(1 + |x_i - x_j|^2)^{\gamma(\theta)}$ *unconditional alignment for* $K(\theta) > 0$ *and* $\gamma(\theta) < \gamma_0 \le 1/2$ *for all* θ *.*

[11] J. A. Carrillo, M. Fornasier, G. Toscani, F. Vecil '10; G. Albi, L. Pareschi '13

The distribution of θ



BBGKY hierarchy with uncertainty

Let us define the $N-$particles density function

$$f^{(N)} = f^{(N)}(\theta, x_1, v_1, \dots, x_N, v_N, t),$$

whose total mass is conserved. Hence, its evolution is described by the Liouville equation

$$\partial_t f^{(N)} + \sum_{i=1}^N v_i \cdot \nabla_{x_i} f^{(N)} = -\frac{1}{N}\sum_{i=1}^N \nabla_{v_i} \cdot \sum_{j=1}^N H_{ij}(\theta)(v_j - v_i) f^{(N)},$$

then we define $f^{(1)}(\theta, x_1, v_1)$ and $f^{(2)}(\theta, x_1, v_1, x_2, v_2, t)$ the marginal densities of $f^{(N)}$ and let $f(\theta, x_1, v_1, t) = \lim_{N\to+\infty} f^{(1)}$ and

$$\tilde{f}(\theta, x_1, v_1, x_2, v_2, t) = \lim_{N\to+\infty} f^{(2)} \underbrace{=}_{\text{ansatz}} f(\theta, x_1, v_1, t) f(\theta, x_2, v_2, t).$$

We can prove [12] that $f = f(\theta, x, v, t)$ is a density function solution of

$$\partial_t f + v \cdot \nabla_x f = \nabla_v \cdot [\mathcal{H}[f] f]$$

[12] C. Cercignani, R. Illner, M. Pulvirenti '94; S.-Y. Ha, E. Tadmor '08

MCgPC methods

Similarly to what we have described for the mean-field equations we can consider the gPC approximation of the microscopic system for

$$x_i(\theta,t) \approx x_i^M = \sum_{k=0}^M \hat{x}_{i,k}\Phi_k(\theta), \qquad v_i(\theta,t) \approx v_i^M = \sum_{k=0}^M \hat{v}_{i,k}\Phi_k(\theta)$$

for which we obtain the following polynomial chaos expansion for all $h = 0,\dots,M$

$$\begin{cases} \dot{\hat{x}}_{i,h} = \hat{v}_{i,h}, \\ \dot{\hat{v}}_{i,h} = \dfrac{1}{N}\displaystyle\sum_{j=1}^N \sum_{k=0}^M e_{hk}^{ij}(\hat{v}_{j,k} - \hat{v}_{i,k}), \quad e_{hk}^{ij} = \dfrac{1}{\|\Phi_h(\theta)\|^2}\displaystyle\int_{\mathbb{R}^{d_\theta}} H_{ij}\Phi_h(\theta)\Phi_k(\theta)d\rho(\theta) \end{cases}$$

and therefore in the limit $N \to +\infty$ the distribution f^M is solution of the mean field problem

$$\partial_t f^M + v\cdot\nabla_x f^M = \nabla_v \cdot [\mathcal{H}[f^M]f^M]$$

MCgPC methods

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for which we obtain the following polynomial chaos expansion for all $h = 0,\dots,M$

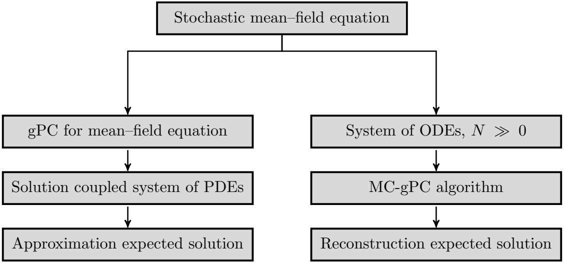
$$\begin{cases} \dot{\hat{x}}_{i,h} = \hat{v}_{i,h}, \\ \dot{\hat{v}}_{i,h} = \dfrac{1}{|S_i|}\displaystyle\sum_{j\in S_i}\sum_{k=0}^{M} e_{hk}^{ij}(\hat{v}_{j,k} - \hat{v}_{i,k}), \quad |S_i| = S \end{cases}$$

and therefore in the limit $N \to +\infty$ the distribution f^M is solution of the mean field problem

$$\partial_t f^M + v \cdot \nabla_x f^M = \nabla_v \cdot [\mathcal{H}[f^M] f^M]$$

MCgPC methods

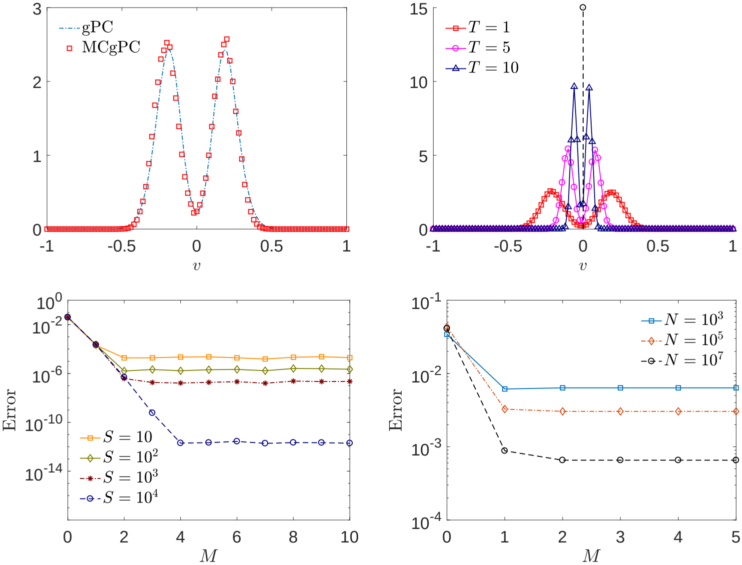
Instead of a cost $O(M^2N^2)$ we then achieve the strongly decreased cost $O(M^2SN)$, $S \ll N$. The expected solution is then reconstructed from expected positions and velocities of the microscopic gPC system. [13]



The MCgPC method is still spectrally accurate in the stochastic variable θ provided we have a smooth dependence of the particle solution from the random field.

[13] J. A. Carrillo, L. Pareschi, M. Z. '18

Validation


gPC
MCgPC
v
$T = 1$
$T = 5$
$T = 10$
v
Error
$S = 10$
$S = 10^2$
$S = 10^3$
$S = 10^4$
M
Error
$N = 10^3$
$N = 10^5$
$N = 10^7$
M

Example 1: 1D & 2D Flocking

Example 2: Mill

Conclusion

- In many equations for the description of the collective dynamics we need to include the effects of uncertainty since at most we have statistical information on the parameters characterizing the interactions.
- For kinetic models, the construction of numerical schemes which are capable to guarantee highly accurate steady states description, positivity and entropy dissipation is essential to have a correct description of the dynamics.
- Stochastic Galerkin methods are spectrally accurate in the random field but may lead to the loss of important structural properties of the numerical solution of VFP equations. Micro-macro schemes have been designed to preserve the large time behavior.
- Monte Carlo gPC (MCgPC) methods are spectrally accurate in the random field and permit to ensure the positivity of statistical quantities.
- **Future research directions**
    - Optimal control in the presence of uncertainty
    - MCgPC for the diffusive models and for the Boltzmann equation with uncertainties
    - Hydrodynamic limit with uncertainty
    - ...