# Report on BIRS workshop, Emergent behaviour in multi-particle systems with non-local interactions
## 22-27 January, 2012

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## 1 Introduction

Collective group behaviour is a fascinating natural phenomenon that is observed at all levels of the animal kingdom, from beautiful bacterial colonies, insect swarms, fish schools and flocks of birds, to complex human population patterns. The emergence of very complex behaviour is often a consequence of individuals following very simple rules, without any external coordination. In recent years, many models of group behaviour have been proposed that involve nonlocal interactions between the species [1, 2, 3, 4]. Related models also arise in a number of other applications such as granular media [5, 6, 7, 8], self-assembly of nanoparticles [9, 10], and molecular dynamics simulations of matter [11].

Due to their nonlocal nature, these systems can exhibit complex and novel phenomena that pose challenging questions and motivate the development of new mathematical techniques. They typically lead to coherent and synchronized structures apparently produced without the active role of a leader in the grouping, phenomena denominated self-organization [12, 13], and it has been reported even for some microorganisms such as myxobacteria [14].

Most of these models are based on discrete models [1, 2, 3, 15] incorporating certain effects that we might call the "first principles" of swarming. These first principles are based on modelling the "sociological behavior" of animals with very simple rules such as the social tendency to produce grouping (attraction/aggregation), the inherent minimal space they need to move without problems and feel comfortably inside the group (repulsion/collisional avoidance) and the mimetic adaptation or synchronization to a group (orientation/alignment). They model animals as simple particles following certain microscopic rules determined by their position and velocity inside the group and by the local density of animals. These rules incorporate the "sociological" or "behavioral" component in the modelling of the animals movement. Even if these minimal models contain very basic rules, the patterns observed in their simulation and their complex asymptotic behavior is already very challenging from the mathematical viewpoint. These 3-zone models are classical in fish modelling [16, 17].

The source of this tendency to aggregation can also be related to other factors rather than sociological as survival fitness of grouping against predators, collaborative effort in food finding, etc. Moreover, we can incorporate other interaction mechanisms between animals as produced by certain chemicals, pheromone trails for ants, the interest of the group to stay close to their roost, physics of swimming/flying, etc. Although the minimal models based on "first principles" are quite rich in complexity, it is interesting to incorporate more effects to render them more realistic, see [13, 18, 19, 20] for instance.

There have been several micro and macroscopic models during the recent years that have attracted a lot the attention of mathematicians as the nonlocal models [21, 22, 23, 24] including Morse potentials, [25, 26, 27] for self-propelled particles with attraction and repulsion effects, and the simple model of alignment in [28]. For instance, the authors in [26] classify the different "zoology" of patterns: translational invariant flocks, rotating single and double mills, rings and clumps; for different parameter values. On the other hand, in the simpler alignment models [28], we get generically a flocking behavior. Much more elaborated models starting from these basic bricks are capable of simulating the collective behavior in case of analyzing systems with a large number of agents $N$. Control of large agent systems are important not only for the somehow bucolic example of the animal behavior but also for pure control engineering for robots and devices with the aim of unmanned vehicle operation and their coordination, see [29, 30] and the references therein.

When the number of agents is large, the use of continuum models for the evolution of a density of individuals becomes essential. Some continuum models were derived phenomenologically [21, 31, 32] including attraction-repulsion mechanisms through a mean force and spatial diffusion to deal with the anti-crowding tendency. Other continuum models are based on hydrodynamic descriptions [33, 34] derived by means of studying the fluctuations or the mean-field particle limits. Hyperbolic systems have also been proposed [35, 36, 37]. The essence of the kinetic modelling is that it does connect the microscopic world, expressed in terms of particle models, to the macroscopic one, written in terms of continuum mechanics systems. A very recent trend of research has been launched in this direction in the last few years, see for instance [38, 39, 34, 40, 41, 42, 43, 44] for different kinetic models in swarming. Introducing noise in these models can lead to phase transitions, a line of research which is wide open [1, 45, 46, 47].

Finally, variational approaches have been very fruitful to attack steady states and their stability for first order models of swarming. A very classical model in this field is the Patlak-Keller-Segel model for chemotactic cell movement [48]. Lots of exciting developments have happened in this direction in the last years [49, 50, 51, 52] and these variational tools have had nice implications in the theory of first order models [53, 54]. Fluid mechanics techniques have also been adapted to the aggregation equation to deeply analyse qualitative properties [55, 56, 57].

The common feature of these models is that they all lead to some non-locality in the equations, either in the form of a large system of ODE's with global coupling, or as a PDE with non-local kernels (integral terms). The analysis, asymptotic behavior, numerical simulation, pattern formation and their stability in many of these models still remain unexplored research territory. The development of these models has in part been motivated by increased use of computers which allows for easy experimentation. In many of these models, novel and exciting phenomena have been observed numerically. However, the fundamental understanding of observed patterns and their dynamics has been lagging. The time is ripe for development of better analytical tools which would allow to gain a better insight of these models.

# 2 Presentation highlights

Several important themes were identified during the workshop. The presentations are loosely classified according to one of the topics below.

## 2.1 Aggregation models

One of the simplest models of interacting particles that yields very complex dynamics is

$$\frac{d}{dt}x_i = \frac{1}{N}\sum_{j\neq i}^{N} F(|x_i - x_j|)\frac{x_i - x_j}{|x_i - x_j|}. \tag{1}$$

where $F(r)$ models the interaction force between the particles [58]. In the hydrodynamic limit $N \to \infty$, the model yields an intergro-differential equation

$$\rho_t + \nabla_x \cdot (\rho v) = 0; \qquad v(x) = \int_{\mathbb{R}^d} F\left(|x-y|\right)\frac{x-y}{|x-y|}\rho(y)dy. \tag{2}$$

The study of aggregation models has been a very active area of research over the past decade; there are by literaly hunderds of papers on this model and its variations; see for example [59, 24, 21, 31] and references therein. Many of the participants talked about the aggregation model and its variations.

Balague discussed recent results on solutions that concentrate uniformly on a sphere, under the power law attractive-repulsive forces. Sharp conditions that establish stability under radial perturbations were given.

Bernoff studied equilibrium configurations of swarming biological organisms subject to exogenous and pairwise endogenous forces. Under certain conditions on the interaction force, the equilibria results in a compactly-supported density. In two-dimensions he showed that the Morse Potential and other "pointy" potentials can generically lead to inverse square-root singularities in the density at the boundary of the swarm support.

Bertozzi gave an introduction to the interesting phenomena of swarming and to the open problems in this area. She reviewed numerical and analytical results for both kinematic and dynamic aggregation equations. She discussed how models are constructed and the emergence of phenomenological behavior for different types of models including flocking, milling, and other patterns. She then presented some results on well-posedness of aggregation equations including a sharp condition on blowup from smooth initial data.

Fellner highlighed the differences between discrete stochastic and continuum versions of the model.

Fetecau discussed the dynamics and equilibria for swarms in the case where the repulsion is Newtonian and attraction is a power law. In many special cases, dynamics and equilibria can be explicitly described. The equilibria have biologically relevant features, such as finite densities and compact support with sharp boundaries. In a related talk, Huang presented some recent results on the asymptotics of the steady states for some of the limiting cases of the power attraction.

Pavlovski and Kolokolnikov presented recent results asymptotics of complex patterns in two and three dimensions. They discussed the patterns that consist of small multiple spots and of a thin ring. These patterns can be understood in terms of stability and perturbations of "lower-dimensional" patterns. Asymptotic methods provide a powerful tool to describe the stability, shape and precise dimensions of these complex patterns.

Laurent's lecture was on the dynamics of aggregation patchs in the case of purely Newtonian kernel. Numerical simulations as well as some exact solutions show that the time evolving domain on which the patch is supported typically collapses on a complex skeleton of codimension one. Reversing the time, any bounded compactly supported solution converges toward a spreading circular patch. A rate of convergence which is sharp in 2D was derived.

Raoul discussed the impact of the singularity of the interaction potential at the origin on the solutions. Some results in one dimension were presented and open questions for higher dimensions were posed.

Bedrossian talked about global existence and finite time blow-up for the critical Patlak-Keller-Segel (PKS) Models with inhomogeneous diffusion. The $L^1$-critical parabolic-elliptic PKS system is a classical model of chemotactic aggregation in micro-organisms well-known to have critical mass phenomena. In this talk, he studied this critical mass phenomenon in the context of PKS models with spatially varying diffusivity of the chemo-attractant in three dimensions and higher. The critical mass is identified to depend only on the local value of the diffusivity and finite time blow-up results show it to be sharp under certain conditions. The methods also provide new blow-up results for homogeneous problems, showing that there exist blow-up solutions with arbitrarily large (positive) initial free energy.

Yao gave a talk on the asymptotics of the blow-up behaviour and radial solutions for the PKS model. Numerically, three types of blow-up behaviour were identified: self-similar with no mass concentrated at the core, imploding shock solution and near-self-similar blow-up with a fixed amount of mass concentrated at the core. She also presented some theoretical results concerning the asymptotic behavior of radial solutions when there is global existence.

## 2.2 Second order models

Models of self-propelled particles typically take acceleration as well as self-propulsion of particles into account. An example of such a model is [26],

$$\frac{d}{dt}v_i = \left(\alpha - \beta\,|v_i|^2\right)v_i + \sum_{j\neq i} F(|x_i - x_j|)\frac{x_i - x_j}{|x_i - x_j|}; \qquad \frac{d}{dt}x_i = v_i$$

where $F(r)$ is models the interaction force between the particles and the term $\left(\alpha - \beta\,|v_i|^2\right)v_i$ is the self-propulsion force. These models typically lead to complex dynamics including swarms, mills and double mills [26, 33, 34, 27]. A related model is the Cucker-Smale equations modelling the flocking of birds [28]; in its simplest form it is

$$\frac{d}{dt}v_i = \frac{\lambda}{N}\sum_{j=1}^{N}\frac{1}{(1+|x_i - x_j|)^{\beta}}\,(v_j - v_i)\,; \qquad \frac{d}{dt}x_i = v_i.$$

Many presentations at the conference discussed recent results for 2nd order models.

Carrillo presented an overview of 2nd order models for swarming. He gave several examples of the derivation by means of kinetic theory arguments of kinetic equations for swarming. One example is the self-propelled particles model. Starting from the particle model, one can construct solutions to a Vlasov-like kinetic equation for the single particle probability distribution function using distances between measures. Another example is the continuous kinetic version of flocking by Cucker and Smale. The large-time behavior of the distribution in phase space is subsequently studied by means of particle approximations and a stability property in distances between measures. A continuous analogue of the theorems of Cucker-Smale will be shown to hold for the solutions on the kinetic model.

Forgoston considered self-propelling agents in the presence of both noise and delay. Delay in the swarm induces a bifurcation that depends on the size of the coupling amplitude. There are several spatio-temporal scales of these swarm structures. The interplay of coupling strength, time delay, noise intensity, and choice of initial conditions can affect the swarm in complicated ways.

Stephan Martin presented the usual self-propelled particle system, but where the morse force was replaced by a quasi-morse potential, having similar properties as the Morse force, but more amenable to analysis. He then explicitly computed the stationary states in the form of rotating flocks. Simulations were also performed which agreed with the explicit analytical solution, and illustrate the parameter dependencies.

Lega presented results of molecular dynamics simulations of disks moving in a two-dimensional box and interacting through special collisions [60]. Because this work was motivated by the existence of complex behaviors in colonies of bacteria, the particles also reorient themselves at random times, thereby simulating bacterial tumbles and inputing energy into the system. She showed that at low packing fractions clusters dynamically form and break up and that, as the packing fraction increases, groups of increasingly larger size are observed, in which the particles move coherently. Such behaviors are markedly different from those observed in systems of particles interacting through elastic collisions.

Frouvelle's talk was on the variation of the Viscek model which describes the alignment and self-organisation in large systems of self-propelled particles. He considered a time-continuous version of this model, in the spirit of the one proposed by P. Degond and S. Motsch, but where the rate of alignment is proportional to the mean speed of the neighboring particles. In the hydrodynamic limit, this model undergoes a phase transition phenomenon between a disordered and an ordered phase, when the local density crosses a threshold value. The two different regimes lead to two distinct macroscopic limits, namely a nonlinear diffusion equation for the density, and a first-order non-conservative hydrodynamic system of evolution equations for the local density and orientation.

Panferov discussed phase transitions in models of Vlasov-McKean type. These equations provide a mean-field description of a system of interacting particles through a pairwise potential V. If the Fourier transform of V has a negative minimum, the system has a critical threshold for the diffusion constant beyond which the trivial uniform steady state becomes unstable and the system experiences a phase transition. He showed that a large class of interactions, when the size of the domain is sufficiently large, the transition is always discontinuous and is characterized by coexistence of several stable states in a certain interval of parameter space.The transition is also shown to occur at a value of the diffusion constant strictly greater than the critical threshold. He also presented the results of a numerical study on the character of phase transition in Vicsek like models of flocking, in which a similar discontinuous transition is observed.

Agueh discussed the adding several forces to Cucker-Smale model to make it more realistic. Namely, the basic C-S model leads to unconditional flocking of all the birds in the swarm. Agueh presented generalizations of the C-S model to include scenarios where a typical bird is subject to a friction force driving it to fly at optimal speed, a repulsive short-range force to avoid collisions, an attractive "flocking" force which takes into account a cone of vision of the bird, and a boundary force to bring the bird back inside the swarm if it is on the edge flying outward. Unlike toe original C-S model, which has the feature that all birs flock to a swarm, simulation of the modified model show that the breakup of a swarm does occur.

A related talk by Seung-Yeal Ha was about asymptotic formation of multi-clusters for the Cucker-Smale and Kuramoto models, and the related phenomenon of synchronization. He derived sufficient conditions for the multi-cluster formation to the particle and kinetic Cucker-Samle and Kuramoto models.

Alethea Barbaro discussed the C-S model with friction and noise. She analysed the existence of phase transitions as one increased the noise or friction coefficients. She found three steady-state solutions for small noise, while only one steady state was found for larger values of noise.

Motsch talked about a model of flocking with asymmetric interactions which aims at improving the C-S model. The C-S model relies on a simple rule: the closer two individuals are, the more they tend to align with each other. In the new model proposed, the strength of the interaction is also weighted by the density: the more an agent is surrounded, the less he will be influenced. As a consequence, interactions between agents are no longer symmetric. It was found that that the dynamics converges to a flock provided that the interaction function decays slowly enough.

Jesus Rosado discussed the well-posedness of the kinetic version of the Cucker-Smale model for flocking. He showed that the unconditional flocking result that Cucker and Smale showed for the particle model also holds in the new framework. He also duscussed some extensions of the kinetic model.

## 2.3 Applications in biology

De Vries and Eftimie described two related models on how various communication mechanisms between species can lead to the formation of biological aggregations. Eftimie presented a nonlocal hyperbolic model in one space dimension which incorporates social interactions among the species with orientation. She computed the speeds at which the organisms travel through the media, as a function of their nonlocal interactions. She discussed the role of communication mechanisms and social interactions on the choice of movement direction of travelling groups. De Vries talk extended the hyperbolic model to a particle-based setting using a system of ODE's instead of a hyperbolic PDE. Many rich dynamics that appear in the hyperbolic model, such such as travelling pulses, zigzag pulses, breathers, and feathers, are also observed in the individual-based models.

Doron Levy discussed recent results on modeling phototaxis in order to understand the functionality of the cell and how the motion of individual cells is translated into emerging patterns on macroscopic scales.

Birnir introduced a dynamic energy budget theory to model the to model the physiology of animals and how it influences their interactions with the environment. This theory was motivated by the study of Icelandic capelin, and helps to explain how changes in physiology can trigger entirely different group behavior influencing migration patterns over large distances.

Einarsson discussed two applications: the role of noise in modelling schooling fish, and modelling biofilm growth using cellular automata. Both models are non-deterministic, but give rise to complex structures. The model reproduces biofilm development in the form of flat biofilms, ripples, streamers, towers, mushroom growth etc.

Rodriguez discussed traveling wave solutions for a Reaction-Diffusion system for crime patterns. This system of equations can be divided into three regimes, which lead to one, two, or three steady-states solutions. There is also an invasion phenomenon of crime hotspots via traveling wave solutions in one dimension.

## 2.4 Applications in engineering and science

In engineering context, multi-particle systems model inter-agent interactions. Typically, these agents can be robots, vehicles, soldiers etc, that need to interact collectively to perform a desgnated task. There is a strong interplay between the mathematical models on one hand and engineering applications on the other. Several speakers gave a talk from a more applied perspective. The diversity of topics illustrate the vitality of the subject.

Gazi talked about the stability of swarms with second order agent dynamics. The inter-agent interactions in the individual based swarm model are provided with artificial potential functions. In this context, he discussed aggregation, social foraging, and formation control.

Lindsay presented some recent results on a singularity formation problem in a nonlinear fourth order PDE modelling a Micro-Elcetro Mechanical Systems (MEMS) Capacitor. The singularity is observed to form in multiple locations within the domain with these locations exhibiting an analyzable dependence on the model parameters and the geometry of the domain. He outlined an asymptotic method which can predict the location(s) where singular solutions form based on the geometry of the domain and the parameters of the system. The theory was demonstrated on several examples.

Ward used asymptotic methods to compute the mean first passage time (MFPT) for a Brownian particle in a three-dimensional domain that contains $N$ small non-overlapping absorbing windows on its boundary. This problem has wide applications in cellular biology where it may be used as an effective first order rate constant to describe, for example, the nuclear export of messenger RNA molecules through nuclear pores. Using detailed analytical properties of a surface Green's function, a three-term asymptotic approximation for the MFPT for the unit sphere was computed. The third term in this expansion depends explicitly on the spatial arrangement of the absorbing windows on the boundary of the sphere. The MFPT is minimized for particular trap configurations that minimize a certain discrete variational problem, which is closely related to the well-known optimization problem of determining the minimum energy configuration for $N$ repelling Coulomb charges on the unit sphere.

Putkaradze gave a lecture titled "Molecular monolayers as interacting rolling balls: crystals, liquid and vapor". Molecular monolayers, especially water monolayers, are playing a crucial role in modern science and technology. He considered simplified models of monolayer dynamics, consisting of rolling self-interacting particles on a plane with an off-set center of mass and a non-isotropic inertia tensor. He further assumed that the physical properties to be the similar to water molecules. The standard tools of statistical mechanics do not apply: for example the system exhibits two temperatures – translational and rotational– for some degrees of freedom, and no temperature can be defined for other degrees of freedom. In spite of apparent simplicity, the behavior of the system is surprisingly rich. Many phenomena were investaged. As a first step towards continuous theory, he presented a Vlasov-like kinetic theory for a gas of rolling balls.

### 2.5 Stochastic models

Most systems in nature have a random component to them. The presence of noise is often one of the driving forces that can completely alter the behaviour of the system. Many presentations at the workshop dealt with the effect on noise on the model.

D'Orsogna's talk was about stochastic nucleation and growth of particle clusters. These model the binding of individual components to form composite structures and is an ubiquitous phenomenon within the sciences. Mean field descriptions lead to well known Becker Doering equations. In cellular biology, however, nucleation events often take place in confined spaces, with a finite number of components, so that discreteness and stochastic effects must be taken into account. She considered a fully stochastic master equation, solved via Monte-Carlo simulations and via analytical insight. This resulted in striking differences between the mean cluster sizes obtained from our discrete, stochastic treatment and those predicted by mean field treatments. Further applications to first passage time results and prion unfolding and clustering dynamics were considered.

Erban discussed three different stochastic methods for spatio-temporal modelling in cellular and molecular biology. The connections between these models and the deterministic models (based on reaction-diffusion-advection partial differential equations) were also presented. He also discussed a hybrid modelling of chomtaxis where an individual-based model of cells is coupled with PDEs for extracellular chemical signals.

Liébana presented a kinetic theory two-species coagulation. He we derived a kinetic theory that approximately describes the process dynamics and determine its asymptotic behavior. Analytical results and direct numerical simulations of the stochastic process both corroborate its predictions and check its limitations.

Haskovec presented two individual based models where social phenomena emerge purely from random behaviour of the agents, without introducing any deterministic "social force" that would push the system towards its organized phase. Instead, organization on the global level results merely from reducing the individual noise level in response to local organization, which is induced by stochastic fluctuations. The first model describes the recently experimentally observed collective motion of locust nymphs marching in a ring-shaped arena and is written in terms of coupled velocity jump processes. The second model was inspired by observations of aggregative behaviour of cockroach nymphs in homogeneous environments and is based on randomly moving particles with individual diffusivities depending on the perceived average population density in their neighbourhood. He showed that both models have regimes leading to global self-organization of the group (synchronization and aggregation). He derived the mean-field limits for both models, leading to PDEs with nonlocal nonlinearities.

Wennberg considered two models of biological swarm behavior. In these models, pairs of particles interact to adjust their velocities one to each other. In the first process, called 'BDG', they join their average velocity up to some noise. In the second process, called 'CL', one of the two particles tries to join the other one's velocity. He established the master equations and BBGKY hierarchies of these two processes. The resulting kinetic hierarchy for the CL process does not satisfy chaos propagation. Numerical simulations indicate the same behavior for the BDG model.

# 3 Outcome of the meeting

The BIRS workshop was a timely opportunity to gather foremost experts on the subject who presented many recent results on multi-particle systems. Several senior participants also gave an overview of the "state of the art" of the field. Mathematically, the two main approaches is to study multi-particle systems using the theory of dynamical systems; or by taking the continuum limit, which typically results in a PDE system that involves integral terms. Due to nonlocal nature, these systems often lead to novel phenomena that have motivated the development of new mathematical tools and pose new problems that were further explored by many participants of this workshop.

As a companion to this workshop, a special issue of Physica D dedicated to multi-particle systems is currently in production, and we expect the publication to appear in early 2013. Many of the participants from this workshop, as well some researchers who did not attend have contributed papers to this special issue. The vitality of this area of research can be demonstrated based on the interesting results obtained in the last year since this conference took place, for instance [61, 62, 63, 64, 65, 66, 67, 68, 69]. Even some of them are direct result of the interactions produced during this meeting.

The diversity of the topics involved and the backgrounds of the participants attest to the vitality of this exciting area which is currently undergoing an explosive development.

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