Lecture 2
Mathematical Tools
of the Kinetic Theory of Active Particles

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Five Lectures

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From a Mathematics of Living Systems

to Modeling Virus Pandemics

P.1. Plan of the Lectures

Nicola Bellomo **Lecture 1. A Quest Towards a Mathematical Theory of Living Systems**

Diletta Burini **Lecture 2. Mathematical Tools of the Kinetic Theory of Active Particles**

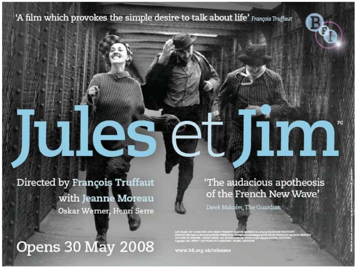
Nicola Bellomo, Diletta Burini and Nisrine Outada **Lecture 3. Towards a Mathematical Theory of Virus Pandemics - Models with Mutations, Variants and Vaccination Programs**

Damian Knopoff **Lecture 4. Heterogeneity and Networks**

Pietro Terna **Lecture 5. Agent Methods to Modeling Virus Pandemics - A quick reference to complexity**

Pietro Terna **Closure, Description of the material support to the Lectures, Acknowledgments**

2.1. On the kinetic theory of active particles



This Lecture is devoted to the derivation of mathematical structures consistent with the strategy proposed in Lecture 1. These can capture the complexity features of living systems. We refer to large systems of very many interacting entities which might be grouped into the so-called functional subsystems.

A key feature of the structure is that interactions have a nonlinearly additive character.

Scaling and selection of the modeling scale

• The representation and modeling of dynamical systems can be developed at the three classical scales: *microscopic* (individual based), *macroscopic* (hydrodynamical), *mesoscopic* (kinetic).

• The dependent variable in the micro- and macro-scale is deterministic, while in the kinetic theory approach it is a probability distribution function over the microscopic state of the interacting entities.

• We focus on the collective dynamics of large systems of interacting individuals. Therefore the kinetic theory approach appears to be the most appropriate to be selected.

• A key difficulty is that the number of interacting entities is not large enough to fully justify the continuity assumption of the distribution function.

2.3. On the kinetic theory of active particles

Pioneering papers and books

* I. Prigogine and and R. Herman, **Kinetic Theory of Vehicular Traffic**, Elsevier, New York, (1971).

* S. Paveri Fontana, On Boltzmann like treatments for traffic flow, *Transp. Research*, 9, 225–235, (1975).

* E. Jager and L.A. Segel, On the distribution of dominance in a population of interacting anonymous organisms, *SIAM J. Appl. Math.* 52, 1442–1468, (1992).

* N. Bellomo and G. Forni, Dynamics of tumor interactions with the host immune system, *Math. Comp. Model.*, 20, 107–122, (1994).

2.4. On the kinetic theory of active particles

Books and surveys on the kinetic theory of active particles

* A. Bellouquid and M. Delitala, **Modelling Complex Biological Systems - A Kinetic Theory Approach**, Birkhäuser-Springer, N.Y., (2006).

* N. Bellomo, A. Bellouquid, L. Gibelli, and N. Outada, **A Quest Towards a Mathematical Theory of Living Systems**, Birkhäuser-Springer, New York, (2017).

* N. Bellomo, D. Burini, G. Dosi, L. Gibelli, D. Knopoff, N. Outada, P. Terna, and M.-E. Virgillito. What is life? A perspective of the mathematical kinetic theory of active particles, *Math. Models Methods App. Sci.*, 31, 1821–1866, (2021). (Open Source)

- This open source essay is the main reference for this lecture.

2.5. On the kinetic theory of active particles

We consider a large system of active particles in the case of spatial homogeneity

• The overall state of the system is subdivided into ***functional subsystems*** (in short FS) labeled by the subscript i. Their state is delivered by the ***one-particle distribution function***

$$f_i = f_i(t, \mathbf{u}) \; : \quad [0, T] \times D_{\mathbf{u}} \to \mathbf{R}_+,$$

such that $f_i(t, \mathbf{u})\, d\mathbf{u}$ denotes the number of ***active particles*** whose state, at time t, is in the interval $[\mathbf{u}, \mathbf{u} + d\mathbf{u}]$ of the i-th functional subsystem.

• $\mathbf{u}$ is the ***vector activity variable*** which models the strategy expressed by each functional subsystem.

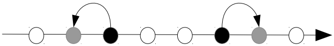
2.6. On the kinetic theory of active particles

Interactions by evolutionary stochastic games: Living entities, at each interaction, *play a game* with an output that depends on their strategy often related to surviving and adaptation abilities.

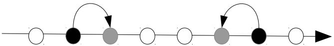
1. **Competitive (dissent):** One of the interacting particles increases its status by taking advantage of the other, obliging the latter to decrease it. Competition brings advantage to only one of the two.
2. **Cooperative (consensus):** The interacting particles exchange their status, one by increasing it and the other one by decreasing it. Interacting active particles show a trend to share their micro-state.
3. **Learning:** One of the two modifies, independently from the other, the micro-state. It learns by reducing the distance between them.
4. **Hiding-chasing:** One of the two attempts to increase the overall distance from the other, which attempts to reduce it.

2.7. On the kinetic theory of active particles

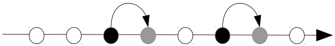
Pictorial illustration of interactions: Black and grey bullets denote, respectively, the pre- and post-interaction states.



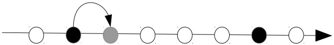
(a) Competition



(b) Cooperation



(c) Hiding-chasing



(d) Learning

2.8. On the kinetic theory of active particles

Stochastic game theory

- *Stochastic game theory deals with entire population of players, where strategies with higher payoff might spread over the population.*
- *The strategy expressed by individuals. i.e. active particles, is heterogeneously distributed over players.*
- *Players are modeled as random variables linked to a distribution function over the activity variable.*
- *The pay-off is heterogeneously distributed over players and it can be motivated by "rational" or even "irrational" strategies.*
- *The payoff depends on the actions of the co-players as well as on the frequencies of interactions. Both quantities depend on the overall state of the system.*

Modeling interactions

- Each a-particle has a sensitivity Ω. The size of Ω depends on the amount of information which can be obtained by an active particle.
- Interactions are nonlinearly additive and are of two types *micro-micro* or *micro-macro*, where the term *macro* corresponds to macroscopic quantities obtained by weighted, by $\mathbf{u}$, averaging of the distribution function.
- Interactions occur with an interaction rate which depend on the distribution function and are related to the *collective learning dynamics*.
- Interactions *can modify the micro-state* of the interacting a-particles and promote *transitions across FSs*.

2.10. On the kinetic theory of active particles

Some remarks on the modeling of interactions

Active particles which play the game: We consider three types of particles: Test particle which is representative of the whole system for each FS; Candidate particles which by interaction with Field particles can acquire state of test particles. The identification of these a-particles is in the sense of statistics, namely by their distribution function over the micro-state.

Interactions can be non-symmetric: Interaction of test (or candidate) particles with field particles involve only those particles which are in their domain of the space of micro-states. However, the dynamics of interaction may not involve the whole domain, but only of a part of it which might not be symmetric. The resulting action of a given number of entities (field entities) over a single one (test entity) cannot be assumed to merely consisting in the linear superposition of the actions exerted individually by all single field entities.

2.11. On the kinetic theory of active particles

Interaction rates

H.1. Micro-micro interaction rates: Candidate (or test particles), of the h-FS and with state $\mathbf{u}_*$ (or $\mathbf{u}$), interact with the field particles, of the k-FS, in the interaction domain Ω. Interactions occur with the ***interaction rate*** $\eta_{hk}[f_h, f_k](\mathbf{u}_*, \mathbf{u}^*)$ (or $\eta_{ik}[f, f_k](\mathbf{u}, \beta^*)$). The subscripts h and k labels the interacting FSs.

H.2. Micro-macro interaction rates: Candidate (or test particles) of the h-FS and with state $\mathbf{u}_*$ (or $\mathbf{u}$), interact with the the k-FS represented by the mean value $\mathbf{E}_k$. Interactions occur with the ***interaction rate*** $\mu_{hk}[f_h, f_k](\mathbf{u}_*, \mathbf{E}_k)$ (or $\mu_{ik}[f, f_k](\mathbf{u}, \mathbf{E}_k)$).

Transition probability densities. Conservative interactions

H.3. **Micro-micro state and FS transitions:** A candidate particle modifies its state as modeled by $\mathcal{C}^i_{hk}[fh, f_k](\mathbf{u}_* \to \mathbf{u}|\mathbf{u}_*, \mathbf{u}^*)$, which denotes the probability density that a candidate particle of the h-FS with state $\mathbf{u}_*$ reaches the state $\mathbf{u}$ in the i-FS after an interaction with the field particles of the k-FS with state $\mathbf{u}^*$.

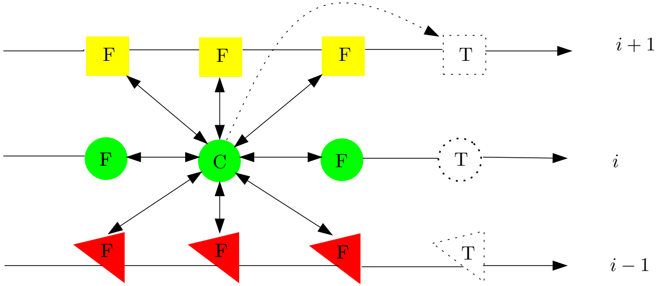
H.4. **Micro-macro state and FS transitions:** A candidate particle modifies its state modeled by $\mathcal{M}^i_{hk}[fh, f_k](\mathbf{u}_* \to \mathbf{u}|\mathbf{u}_*, \mathbf{u}^*)$, which denotes the probability density that a candidate particle of the h-FS with state $\mathbf{u}_*$ reaches the state $\mathbf{u}$ in the i-FS after an interaction with the field particles of the k-FS with state $\mathbf{u}^*$.

Proliferative-destructive events.

H.4. **Proliferative dynamics:** A candidate h-particle may proliferate in the i-FS and state $\mathbf{u}$ as modeled by the terms $\mathcal{P}^i_{hk}[f_h, f_k](\mathbf{u}_* \to \mathbf{u}|\mathbf{u}_*, \mathbf{u}^*)$ and $\mathcal{M}^i_{hk}[f_h, f_k](\mathbf{u}_* \to \mathbf{u}|\mathbf{u}_*, \mathbf{E}_k)$, corresponding - respectively - to micro-micro and micro-macro interactions, by interaction with the field particles of the k-FS with state $\mathbf{u}^*$ and with the k-FS as a whole.

H.5. **Destructive dynamics:** A test i-particle may destroyed in the i-FS and state $\mathbf{u}$ as modeled by the term $\mathcal{D}_{ik}[f_h, f_k](\mathbf{u}, \mathbf{u}^*)$ and $\mathcal{N}^i_{hk}[f_h, f_k](\mathbf{u}, \mathbf{E}_k)$, corresponding - respectively - to micro-micro and micro-macro interactions, by interaction with the field particles of the k-FS with state $\mathbf{u}^*$ and with the k-FS as a whole.

Pictorial illustration, where green and white bullets denote, respectively, the pre- and post-interaction states.



Balance within the space of microscopic states and structure

Variation rate of the number of active particles

$=$ *Inlet flux rate caused by conservative interactions*

$-$*Outlet flux rate caused by conservative interactions*

$+$*Inlet flux rate caused by proliferative interactions*

$-$*Outlet flux rate caused by destructive interactions*,

where all above fluxes include both micro-micro and micro-macro interactions, as well as the dynamics of mutations.

This balance relation corresponds to the following structure:

$$\partial_t f_i(t, \mathbf{u}) = \big(\mathcal{C}_i + \mathcal{M}_i - \mathcal{L}_i - \mathcal{L}_i^M + \mathcal{P}_i - \mathcal{D}_i + \mathcal{P}_i^M - \mathcal{D}_i^M\big)[f_h, f_k](t, \mathbf{u}).$$

Calculations toward a mathematical structure

$$\mathcal{C}_i = \sum_{h,k=1}^{n} \int_{\Omega\times\Omega} \eta_{hk}[\cdot]\mathcal{C}_{hk}^{i}[f_h, f_k]\,(\mathbf{u}_* \to \mathbf{u}|\mathbf{u}_*, \mathbf{u}^*)\, f_h(t, \mathbf{u}_*) f_k(t, \mathbf{u}^*)\, d\mathbf{u}_* d\mathbf{u}^*,$$

$$\mathcal{M}_i = \sum_{h,k=1}^{n} \int_{\Omega} \mu_{hk}[f_h, f_k]\mathcal{M}_{hk}^{i}[\cdot]\,(\mathbf{u}_* \to \mathbf{u}|\mathbf{u}_*, \mathbf{u}^*)\, f_h(t, \mathbf{u}_*)\mathbf{E}_k(t)\, d\mathbf{u}_*,$$

$$\mathcal{L}_i = f_i(t, \mathbf{u}) \sum_{k=1}^{n} \int_{D_{\mathbf{u}}} \eta_{ik}[f_i, f_k](\mathbf{u}, \mathbf{u}^*)\, f_k(t, \mathbf{u}^*)\, d\mathbf{u}^*,$$

$$\mathcal{L}_i^M = f_i(t, \mathbf{u}) \sum_{k=1}^{n} \mu_{ik}[\cdot](\mathbf{u}, \mathbf{E}_k(t))\, \mathbf{E}_k(t),$$

Calculations toward a mathematical structure:

$$\mathcal{P}_i = \sum_{h,k=1}^{n} \int_{\Omega\times\Omega} \eta_{hk}[f_h, f_k](\mathbf{u}_*, \mathbf{u}^*)\mathcal{P}^i_{hk}(\mathbf{u}_*, \mathbf{u}^*)\, f_h(t, \mathbf{u}_*) f_k(t, \mathbf{u}^*)\, d\mathbf{u}_*\, d\mathbf{u}^*,$$

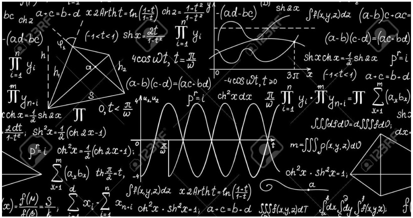
$$\mathcal{D}_i = f_i(t, \mathbf{u}) \sum_{k=1}^{n} \int_{D_{\mathbf{u}}} \mu_{ik}[f_i, f_k](\mathbf{u}, \mathbf{u}^*)\, \mathcal{D}_{ik}(\mathbf{u}, \mathbf{u}^*) f_k(t, \mathbf{u}^*)\, d\mathbf{u}^*.$$

And similarly for proliferative destructive dynamics corresponding to micro-macro interactions.

Remark; The general theory includes space dynamics. See the bibliography in Slide 2.4.

2.18. On the kinetic theory of active particles

We need a mathematics for a “living”, multiscale, evolutionary, nonlinear world



END Lecture 2!