A Multiscale Approach to Cell Movements

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Organs-on-chip and the new medicine





Organs-on-chip and the new medicine





The multiscale approach



• The real goal of these models

- is to use Organs-on-chip to
- predict the behaviour of
- real organs, so on the scale
- of billions of cells, using the
- data from the experiments
- at the microscale
- Create more realistic digital
- twins of our body
- It is crucial to keep the micro
- information in the memory
- of the macro models

A crop of the full chip



Figure: Crop of the microfluid chip after 72 hours

De Ninno A., Bertani F.R., Gerardino A., Schiavoni G., Musella M., Galassi C., Mattei F., Sistigu A., Businaro L. Microfluidic Co-Culture Models for Dissecting the Immune Response in in vitro Tumor Microenvironments. J. Vis. Exp. 170, e61895, doi:10.3791/61895, 2021

Cell trajectories



Cell trajectories performed by WT-cells and KO-type cells

Experiments (see Vacchelli et al: Science.(2015), Businaro et al: Lab on Chip rep.(2014))

- Tumour and KT/WT-type immune cells
- KO-type: uncorrelated random walk
- WT-type: strongly directed movement ⇒ Chemotaxis
- Tumour cells local sources of chemoattractan
- WT-type: Generation of tumour killing agent
- cytokine
- Chemical diffusion

Available Data:

- Tumour and immune cell trajectories
- No information about chemical distribution

The time-lapse of the experiment



- 1702µm × 1361µm
- Duration: 48h-72h
- Cell movement: Diffusion and
- Chemotaxis
- Micro-channels allow only one cell to move through each.



A first macroscopic model



Figure: Numerical domain

Model(2D chamber) modified Keller-Segel model $\frac{\partial}{\partial t}T = D_T \Delta T - \lambda_T(\omega)T - k_T(t)T,$ $\frac{\partial}{\partial t}M = D_M \Delta M - div(M \cdot \chi \nabla) - k_M(t)M,$ $\frac{\partial}{\partial t}\varphi = D_{\varphi}\Delta\varphi + \alpha_{\phi}T - \beta_{\varphi}\varphi,$

$$\frac{\partial}{\partial t}\omega = D_{\omega}\Delta\omega + \alpha_{\omega}M - \beta_{\omega}\omega,$$

 ^{2L}_{x+L} Braun E.C., Bretti G., Natalini R. Mass-Preserving Approximation of a Chemotaxis Multi-Domain Transmission Model for Microfluidic Chips. Mathematics, 9(6)688, 1–34, 2021

A first macroscopic model



Figure: Initial distribution of T_0, M_0, φ_0 and ω_0

- Implicit Crank-Nicolson method for diffusion term
 and source term
- Explicit central discretization for chemotactical convection term
- Articial viscosity for improved stability in presence of high Péclet numbers
- Asymptotic Higher Order schemes(AHO) for the hyperbolic partial dierential equation.
- Numerical boundary conditions that preserve the mass (for no-ux BC).
- Trasmission condition of Kedem-Katchalski type
 (jump for density at interface)

A first macroscopic model



Figure: Initial distribution of T_0, M_0, φ_0 and ω_0

Back to the experimental data



Figure: left: Tracked cell . Right: Artificially created cells.

Beyond Keller-Segel: a micro-hybrid model



Gabriella Bretti, Adele De Ninno, Roberto Natalini, Daniele Peri and Nicole Roselli, Estimation Algorithm for a Hybrid PDE–ODE Model Inspired by Immunocompetent Cancer-on-Chip Experiment, Axioms 2021, 10(4), 243

A hybrid model

 $X_i(t)$: position of the *i*-th cell $\phi(x, t)$: concentration of the chemoattractant





A basic discrete model with chemotaxis

(1)
$$\begin{cases} \dot{x}_i = v_i, \\ \dot{v}_i = \frac{1}{N} \sum_{j=1}^N \gamma(v_i - v_j, x_i - x_j) + \eta \nabla_x \varphi^t(x_i) \\ \partial_t \varphi = D\Delta \varphi - \kappa \varphi + f(x, X(t)) \end{cases}$$

- x_i Position at time t of the i-th cell
- v_i Velocity at time t of the i-th cell
- v_i Velocity at time t of the i-th cell φ Concentration of a chemoattractant produced by the cells $\gamma(v,x)$ Interaction function among the cells
- f(x, X) Production of chemoattractant

Main goals

- Study of the mascroscopic behavior of the dynamical system
- Kinetic approach (Vlasov-type model): density of particles
- Hydrodynamic limit (Euler-type model): density of cells + velocity field:
- a numerical study
- without chemotaxis
- with chemotaxis



The Cucker-Smale model (no chemistry)

(2)
$$\begin{cases} \dot{x}_i = v_i, \\ \dot{v}_i = \frac{1}{N} \sum_{j=1}^N \psi(x_i - x_j)(v_j - v_i) \end{cases}$$

* F. Cucker & S. Smale, Ieee T. Automat. Contr (2007) * S.Y. Ha & J.G. Liu, Commun Math Sci (2009)

$$\psi(\xi) = \left(1 + \frac{\left\|\xi\right\|^2}{R^2}\right)^{-\sigma}$$

time-asymptotic flocking

$$\lim_{t \to +\infty} \sum_{i=1}^{N} \|v_i(t) - v_{\rm CM}(t)\|^2 = 0;$$
$$\sup_{0 \le t \le +\infty} \sum_{i=1}^{N} \|x_i(t) - x_{\rm CM}(t)\|^2 < +\infty$$

The flow

K

The system (2)
$$\begin{cases} \dot{x}_i = v_i, \\ \dot{v}_i = \frac{1}{N} \sum_{j=1}^N \psi(x_i - x_j)(v_j - v_i) \\ \text{Generates a flow } \Phi^t \text{which is, given the initial data } (x^{in}, v^{in}) = (x_1^{in}, \dots, x_N^{in}, v_1^{in}, \dots, v_N^{in}) \\ \Phi^t(x^{in}, v^{in}) = (x(t), v(t)) \end{cases}$$

A first mean field approach: the empirical measures

Given a solution (x(t), v(t)) to system (2). The so-called empirical measure

$$\Pi_{N}^{t}(x,v) := \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_{i}(t)) \delta(v - v_{i}(t))$$

is a special solution to the Vlasov equation:

$$(3)\partial_t \rho^t(x,v) + v \cdot \nabla_x \rho^t(x,v) + \nabla_v \cdot \left(\rho^t(x,v) \int_{2^d} \psi(x-y)(v-w)\rho^t(y,w) dy dw\right) = 0$$

* S.-Y. Ha, E. Tadmor, From particle to kinetic and hydrodynamic descriptions of flocking, Kinet. Relat. Models 1 (2008) 415-435
* Carrillo, José A.; Choi, Young-Pil Mean-field limits: from particle descriptions to macroscopic equations. Arch. Ration. Mech. Anal. 24 (3) (2021) 1529-1573.

The mean field limit: the empirical measures approach

Theorem: given an initial measure ρ^{in} such that $\lim_{N\to\infty} W(\Pi_N^{in},\rho^{in})=0$ then there exist a unique solution ρ^t to

$$\partial_t \rho^t(x,v) + v \cdot
abla_x \rho^t(x,v) +
abla_v \cdot \left(
ho^t(x,v) \int_{2^d} \psi(x-y)(v-w)
ho^t(y,w) dy dw
ight) = 0$$

this solution belongs to $L^{\infty}([0,\infty); \mathcal{P}(\mathbb{R}^{\in d}))$

and

$$\overline{\lim}_{N \to \infty} \sup_{t \in [0,\infty)} W(\Pi_N^t, \rho^t) = 0$$

Seung-Yeal Ha, Jeongho Kim, Xiongtao Zhang, Kinetic & Related Models (2018)

A different approach: Mean field limit by marginals

Idea: considering the movement of a generic particle solution to the Liouville equation associated to an Hamiltonian system

Consider the pushforward by the flow Φ^t of a compactly supported (symmetric by permutations of the variables N-particles) probability density ρ_N^{in} on the phase space

$$\Phi^t \# \rho_N^{in} := \rho_N^t$$

which is the solution to the Liouville's equations associated to the system

$$\begin{array}{l} \partial_t \rho_N^t + V \cdot \nabla_X \rho_N^t + \sum_{i=1}^N \nabla_{v_i} \cdot (G_i \rho_N^t) = 0, \ \rho_N^{t=0} = \rho_N^{in} \\ \\ \text{with} \quad G_i = \frac{1}{N} \sum_{j=1}^N \psi(x_i - x_j)(v_j - v_i) \end{array}$$

Mean field limit by marginals

To describe the movement of a "generic" particle in the limit of diverging number of particles, we want to perform an average on the N particles but one. Then, we take the first marginal to the solution to the Liouville equation

$$\rho_{N;1}^t(x,\xi) := \int_{\mathbb{R}^{2(d-1)N}} \rho_N^t(x,\xi,x_2,\xi_2,\dots,x_N,\xi_N) dx_2 d\xi_2\dots dx_N d\xi_N$$

The marginal approaches the solution to the Vlasov eq.

$$\rho_{N;1}^t(x,\xi) \approx \rho^t$$

A mean field limit with estimate

Theorem 1. R.N. - T. Paul, DCDS-B (2022)

Let Φ^t be the flow generated by the system (2), ψ bounded positive nonincreasing Lipschitz continuous, and let ρ^t be the solution to the Vlasov equation (3) with an initial condition $\rho^{in} \in L^1(\mathbb{R}^{2d})$ compactly supported. Let moreover $\rho_{N;1}^t$ be the first marginal of $\rho_N^t := \Phi^t \#(\rho^{in})^{\otimes N}$. Then, for all N > 1, $t \ge 0$,

$$W_2(\rho_{N;1}^t, \rho^t) \le 4 \|\psi\|_{\infty}^2 (2|\bar{v}| + |supp[\rho^{in}]|) \left(\frac{e^{Lt} - 1}{L}\right)^{\frac{1}{2}} N^{-\frac{1}{2}}$$

with

$$L := 2(1 + 8 \|\psi\|_{\infty}^2 \|v\|_{L^{\infty}(supp[\rho^{in}])}^2) \text{ and } \bar{v} = \int v \rho^{in} dx dv$$

we $\|v\|_{L^{\infty}(supp[\rho^{in}])} := \sup_{v \in V} \|v\|_{\infty}$

where $||v||_{L^{\infty}(supp[\rho^{in}])} := \sup_{(x,v)\in supp[\rho^{in}]} |v|$

The main tool

Theorem 3.6. Let us define the set of compactly supported probability measure on \mathbf{R}^{2dN} invariant by permutation:

$$\mathcal{P}_{c}^{p}(\mathbf{R}^{2dN}) := \{ \rho \in \mathcal{P}_{c}(\mathbf{R}^{2dN}), \rho(\sigma(dZ)) = \rho(dZ), \ \forall \sigma \in \Sigma_{N} \}$$

where $\sigma(Z)$ is defined in (9).

Let us suppose that the two equations

(25)
$$\partial_t \rho_i^t + V \cdot \nabla_X \rho_i^t = \nabla_V \cdot (\mathbf{v}_i([\rho_i^{in}]^{\leq t}, X, V)\rho_i^t), \ \rho_i^0 = \rho_i^{in} \in \mathcal{P}_c^p(\mathbf{R}^{2dN}), \ i = 1, 2,$$

have the property of existence and uniqueness of solutions in $C^0(\mathbf{R}^+, \mathcal{P}_c^p(\mathbf{R}^{2dN}))$. Then, for all $t \in \mathbf{R}^+$, and all i = 1, 2,

$$W_{2}((\rho_{1}^{t})_{N:1}, (\rho_{2}^{t})_{N:1})^{2} \leq e^{\int_{0}^{t} L_{1}(s)ds} W_{2}(\rho_{1}^{in}, \rho_{2}^{in})^{2} \\ + \frac{2}{N} \int_{0}^{t} \int_{\mathbf{R}^{2dN}} |\mathbf{v}_{1}([\rho_{1}^{in}]^{\leq s}, Y, \Xi) - \mathbf{v}_{2}([\rho_{2}^{in}]^{\leq s}, Y, \Xi)|^{2} \rho_{2}^{s}(dY, d\Xi) e^{\int_{s}^{t} L_{1}(u)du} ds$$

with

$$L_1(t) = 2(1 + \sup_{(X,V)\in supp(\rho_1^t)} (\operatorname{Lip}(\mathbf{v}_1(t,X,V))_{(X,V)})^2).$$

Let moreover ρ_i^t , i = 1, 2, be two solutions of the equations (25) and let π_N^t be the unique (measure) solution to the following linear transport equation

 $\partial_t \pi_N + V \cdot \nabla_X \pi_N + \Xi \cdot \nabla_Y \pi_N = \nabla_V \cdot (\mathbf{v}_1([\rho_1^{in}]^{\leq t}, X, V) \pi_N^t + \nabla_\Xi \cdot (\mathbf{v}_2([\rho_2^{in}]^{\leq t}, Y, \Xi) \pi_N^t)$

Lemma A.1. For all $t \in \mathbf{R}$, π_N^t is a coupling between ρ_1^t and ρ_2^t .

Lemma A.2. Let

$$D_N(t) := \frac{1}{N} \int ((X - Y)^2 + (V - \Xi)^2) \pi_N^t (dX dV dY d\Xi).$$

Then

$$\frac{dD_N}{dt} \leq L_1(t)D_N + \frac{1}{N} \int_{]bR^{2dN}} |\mathbf{v}_1(t,Y,\Xi) - \mathbf{v}_2(t,Y,\Xi)|^2 \rho_2^t(dY,d\Xi)$$

Comparison between microscopic and Vlasov

- Flocking case (no chemo)
- (Simulation by Marta Menci)



Comparison between microscopic and Vlasov

Non flocking case (no chemo)

(Simulation by Marta Menci)



Come back to chemotaxis

$$(1) \begin{cases} \dot{x}_i = v_i, \\ \dot{v}_i = \frac{1}{N} \sum_{j=1}^N \gamma(v_i - v_j, x_i - x_j) + \eta \nabla_x \varphi^t(x_i) \\ \partial_t \varphi = D\Delta \varphi - \kappa \varphi + f(x, X(t)) \end{cases}$$

- Non local space-time interaction in the Force field
- The associated solution is no more a flow!
- $\rho_N^t = \Phi_N^t \# \rho_N^{in}$ does not satisfy a closed equation (pseudo-Liouville eq.)

The nonlinear nonlocal Vlasov equation

$$T = \begin{cases} \partial_t \rho^t + v \cdot \nabla_x \rho^t = \nabla_v (\nu(t, x, v) \rho^t), \ \rho^0 = \rho^{in} \in \mathcal{P}(\mathbf{R}^{2d} \\ \nu(t, x, v) = \gamma * \rho^t(x, v) + \eta \nabla_x \psi^t(x) + F_{ext}(x), \\ \partial_s \psi^s(x) = D \Delta_x \psi - \kappa \psi + g(x, \rho^s), \ \psi^0 = \varphi^{in}. \\ g(x, \rho^s) = \chi * \rho^s(x). \end{cases}$$

(V)



The main convergence theorem

<u>Natalini, Roberto; Paul, Thierry The mean-field limit for hybrid models of collective motions with chemotaxis.</u> SIAM J. Math. Anal. <u>55</u>, No. 2, 900-928 (2023)

Theorem 2.1. Let ρ^{in} be a compactly supported probability on \mathbb{R}^{2dN} , let Φ_N^t be the mapping generated by the particles system (3, 4, 5, 6) as defined by (7), and let $\tau_{\rho^{in}}$ be the function defined in formula (41) below.

Then, for any $t \geq 0$,

$$W_2\left((\Phi_N^t \# (\rho^{in})^{\otimes N})_{N;1}, \rho^t\right)^2 \le \tau_{\rho^{in}}(t) \begin{cases} N^{-\frac{1}{2}} & d = 1\\ N^{-\frac{1}{2}} \log N & d = 2\\ N^{-\frac{1}{d}} & d > 2 \end{cases}$$

Moreover, let us denote by $\varphi_{Z^{in}}^t$ the chemical density solution of (3, 4, 5, 6) with initial data (Z^{in}, φ^{in}) and by $\psi_{\rho^{in}}^t$ the one solution of (14, 15, 16, 17) with initial data $(\rho^{in}, \varphi^{in})$. Then

$$\int_{\mathbf{R}^{2dN}} \|\nabla \varphi_{Z^{in}}^t - \nabla \psi_{\rho^{in}}^t\|_{\infty}^2 (\rho^{in})^{\otimes N} (dZ^{in}) \le \tau_c(t) \begin{cases} N^{-\frac{1}{2}} & d = 1\\ N^{-\frac{1}{2}} \log N & d = 2\\ N^{-\frac{1}{d}} & d > 2 \end{cases}$$



Comparison between microscopic and Vlasov with chemotaxis

Non flocking

case

(Simulation by Marta Menci)



The monokinetic situation

Assume now the initial density is monokinetic

$$\rho^{in}(x,v) = \mu^{in}(x)\delta(v - u^{in}(x))$$

Theorem 6.1. Let μ^t, u^t, ψ^t be a solution to the following system

$$\begin{cases} \partial_t \mu^t + \nabla(u^t \mu^t) = 0\\ \partial_t (\mu^t u^t) + \nabla(\mu^t (u^t)^{\otimes 2}) = \mu^t \int \gamma(\cdot - y, u^t(\cdot) - u^t(y)) \mu^t(y) dy + \eta \mu^t \nabla \psi^t + \mu^t F\\ \partial_s \psi^s = D\Delta \psi - \kappa \psi + \chi * \mu^s, \ s \in [0, t],\\ (\mu^0, u^0, \psi^0) = (\mu^{in}, u^{in}, \psi^{in}) \in H^s, \ s > \frac{d}{2} + 1. \end{cases}$$
where $\mu^t, u^t \in C([0, t]; H^s) \cap C^1([0, T]; H^{s-1}), \ \psi^t \in C([0, t]; H^s) \cap C^1([0, T]; H^{s-2}) \cap L^2(0, T; H^{s+1})^3.$
Then $\rho^t(x, v) := \mu^t(x)\delta(v - u^t(x))$ solves the following system
$$\begin{cases} \partial_t \rho^t + v \cdot \nabla_x \rho^t = \nabla_v(\nu(t, x, v)\rho^t),\\ \nu(t, x, v) = \gamma(x, v) * \rho^t + \eta \nabla_x \psi^t(x) + F_{ext}(x), \end{cases}$$

$$\begin{array}{l} \mathcal{D}(t,x,v) = \gamma(x,v) * \rho + \eta \nabla_x \psi(x) + \Gamma_{ext}(x) \\ \partial_s \psi^s(z) = D\Delta_z \psi - \kappa \psi + g(z,\rho^s), \ \psi^0 = \psi^{in}, \\ \rho^0(x,v) = \mu^{in}(x)\delta(v - u^{in}(x)). \end{array}$$

Looking for a good macroscopic model

Marta Menci, Roberto Natalini, Thierry Paul, MICROSCOPIC, KINETIC AND HYDRODYNAMIC HYBRID MODELS OF COLLECTIVE MOTIONS WITH CHEMOTAXIS: A NUMERICAL STUDY, preprint 2023





Nonlocal Valsov equation:

$$\begin{aligned} \partial_t \rho^t + v \partial_x \rho^t &= \partial_v (\nu(t, x, v) \rho^t), \\ \nu(t, x, v) &= \int_2 \frac{v - w}{(1 + |x - y|^2)^\beta} \rho^t(y, w) dy dw + \eta \partial_x \psi^t(x) - \alpha v, \\ \partial_s \psi^s(x) &= D \partial_x^2 \psi - \kappa \psi + \int_{\mathbb{R}} \int_{x - R}^{x + R} \rho^s(y) dy d\xi, \end{aligned}$$

Our nonlocal hydrodinamic equation:

 $\partial_t \mu^t + \partial_x (u^t \mu^t) = 0$

Compare the momenta to the hydrodynamic quantities

$$\nu_0^t(x) = \int \rho^t(x,\xi) d\xi \approx \mu^t(x)$$
$$\nu_1^t(x) = \int \xi \rho^t(x,\xi) d\xi \approx \mu^t(x) u^t(x)$$

$$\partial_t (\mu^t u^t) + \partial_x (\mu^t (u^t)^2) = \mu^t \int \gamma(\cdot - y, u^t(\cdot) - u^t(y)) \mu^t(y) dy + \eta \mu^t \partial_x \psi^t - \alpha \mu^t u^t \\ \partial_s \psi^s = D \partial_x^2 \psi - \kappa \psi + \int_{x-R}^{x+R} \mu^s(y) dy, \ s \in [0, t].$$



The monokinetic case with initial data:

$$\rho^{0}(x,v) = \frac{1}{2\pi\sigma_{x}\sigma_{v}}e^{\frac{-(x-x_{0})^{2}}{2\sigma_{x}^{2}} + \frac{-(v-v_{0})^{2}}{2\sigma_{v}^{2}}}$$



chemotaxis, no damping, t=2: no longer monokinetic

The monokinetic case with initial data:

$$\rho^{0}(x,v) = \frac{1}{2\pi\sigma_{x}\sigma_{v}}e^{\frac{-(x-x_{0})^{2}}{2\sigma_{x}^{2}} + \frac{-(v-v_{0})^{2}}{2\sigma_{v}^{2}}}$$



chemotaxis, damping, t=2: dissipation of energy



The non-monokinetic case with initial data:

$$\rho^{0}(x,v) = \frac{1}{2\pi\sigma_{x}\sigma_{v}}e^{\frac{-x^{2}}{2\sigma_{x}^{2}}}\left(e^{\frac{-(v+v_{0})^{2}}{2\sigma_{v}^{2}}} + e^{\frac{-(v-v_{0})^{2}}{2\sigma_{v}^{2}}}\right) \Longrightarrow u^{0}(x) = 0$$

No chemotaxis No damping t=3

chemotaxis No damping t=7



The Hydrodynamic model with a small pressure term

Our nonlocal hydrodinamic equation with a small pressure (to avoid blow-up)

 $\begin{cases} \partial_t \mu^t + \partial_x (u^t \mu^t) = 0\\ \partial_t (\mu^t u^t) + \partial_x (\mu^t (u^t)^2 + \varepsilon P(\mu^t)) = \mu^t \int \gamma(\cdot - y, u^t(\cdot) - u^t(y)) \mu^t(y) dy + \eta \mu^t \partial_x \psi^t - \alpha \mu^t u^t dy dy + \eta \mu^t \partial_x \psi^t + \alpha \mu^t u^t dy dy + \eta \mu^t \partial_x \psi^t + \eta \mu^t \partial_y \psi^t$

$$\partial_s \psi^s = D \partial_x^2 \psi - \kappa \psi + \int_{x-R}^{x+R} \mu^s(y) dy, \ s \in [0,t].$$

Compare with the Preziosi-Euler model for chemotaxis in vasculogenesis $\begin{cases} \partial_t \mu^t + \partial_x (u^t \mu^t) = 0 \\\\ \partial_t (\mu^t u^t) + \partial_x (\mu^t (u^t)^2 + P(\mu^t)) = +\eta \mu^t \partial_x \psi^t - \alpha \mu^t u^t \\\\ \partial_s \psi^s = D \partial_x^2 \psi - \kappa \psi + \mu^t. \end{cases}$





- The Vlasov model gives a reliable approximation of the microscopic case
- The Hydrodynamic non local model is a good approximation in the monokinetic
- case before blow-up (pressureless gas). And in general the Vlasov remains monokinetic only for short times
- Adding a (small) pressure, in the spirit of Preziosi, takes into account for the neglected momenta, but only for certain values of epsilon.
- Damping, which is a natural ingredient in these models even at the microscopic scale, helps a lot in keeping the hydrodynamics near the kinetic.



Some references

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AUGURI PIERO!



