A Wasserstein gradient flow approach to Poisson-Nernst-Planck equations

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(joint work with D. Kinderlehrer and X. Xu)

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The model : ionic transport (biocells ?)

$$\left\{ \begin{array}{rcl} \partial_t u & = & \Delta u^m + \mathrm{div}\left(u\nabla\left(U+\Psi\right)\right), \\ \partial_t v & = & \Delta v^m + \mathrm{div}\left(v\nabla\left(V-\Psi\right)\right), \\ -\Delta\Psi & = & u-v. \end{array} \right. \qquad t \geq 0,\ x \in \mathbb{R}^d,\ d \geq 3, \qquad \text{(PNP)}$$

Densities $u, v = \pm$ charges (macroscopic), confining external potentials U, V, nonlocal coupling Ψ, nonlinear diffusion $m \geq 1$

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Rmk2 : physical case = bounded domain $\Omega \subset \mathbb{R}^d$ with homogeneous Neumann BC's

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Newton potential

$$-\Delta\Psi = u - v \Leftrightarrow \Psi = (-\Delta)^{-1}[u-v]$$
$$\Leftrightarrow \Psi(x) = G * [u-v](x) = \int_{\mathbb{R}^d} \frac{C_d}{|x-y|^{d-2}}(u-v)(y)\,\mathrm{d}y.$$

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Facts :

1. Positivity $u^0(x), v^0(x) \geq 0 \Rightarrow u(t,x), v(t,x) \geq 0$
2. Conservation of mass $\int_{\mathbb{R}^d} u(t,x)\,\mathrm{d}x = \int_{\mathbb{R}^d} u^0(x)\,\mathrm{d}x$ and $\int_{\mathbb{R}^d} v(t,x)\,\mathrm{d}x = \int_{\mathbb{R}^d} v^0(x)\,\mathrm{d}x$
3. Energy dissipation $\frac{d}{dt}\mathcal{E}(u(t), v(t)) \leq 0$,

$$\mathcal{E}(u,v) = \underbrace{\mathcal{E}_m(u,v)}_{\text{diffusion}} + \underbrace{\int uU + vV}_{\text{potential}} + \underbrace{\frac{1}{2}\int |\nabla\Psi|^2}_{\text{electrostatic}}$$

with

$$\mathcal{E}_m(u,v) = \begin{cases} \int u\log u + v\log v & \text{if } m = 1 \\ \frac{1}{m-1}\int u^m + v^m & \text{if } m > 1 \end{cases}$$

Rmk : $\mathcal{E}_m \underset{m\downarrow 1}{\to} \mathcal{E}_1$ = Boltzmann entropy, unified framework

Wasserstein distance $\mathcal{W}_2$

$$\mathcal{P} = \mathcal{P}^2(\mathbb{R}^d) = \{\rho \geq 0 : \, d\rho(\mathbb{R}^d) = 1, \int |x|^2 \, d\rho(x) < \infty\}$$

Optimal transportation problem [Monge∼1780, Kantorovich∼1950]

$$\boxed{\mathcal{W}_2^2(\rho_0, \rho_1) := \inf_{\gamma \in \Gamma(\rho_0, \rho_1)} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |x - y|^2 d\gamma(x, y)}$$

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Dynamical representation :

Theorem [Benamou-Brenier formula '99]

For fixed endpoints $\rho_0, \rho_1 \in \mathcal{P}$ the interpolation geodesics ρ_t between ρ_0, ρ_1 can be represented by

$$\partial_t \rho_t + \operatorname{div}(\rho_t v_t) = 0,$$

where (ρ_t, v_t) minimize the Lagrangian action

$$A(\rho, v) = \int_0^1 \int_{\mathbb{R}^d} |v_t(x)|^2 \mathrm{d}\rho_t(x) \mathrm{d}t.$$

Moreover $\mathcal{W}_2^2(\rho_0, \rho_1) = \inf A(\rho, v)$.

Riemanian calculus in $\mathcal{P}(\mathbb{R}^d)$ [Otto '99]

$\mathcal{P} =$ manifold $\mathcal{M}$, geodesics $\partial_t \rho_t + \mathrm{div}(\rho_t v_t) = 0$, energy $v_t \in L^2(\mathbb{R}^d, \mathrm{d}\rho_t)$.

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- Tangent plane $T_\rho \mathcal{P} := \{v \in L^2(\mathrm{d}\rho)\}$, Riemanian metric for tangent vectors $s_1 \sim -\mathrm{div}(\rho v_1)$ and $s_2 \sim -\mathrm{div}(\rho v_2)$ in $T_\rho \mathcal{P}$

$$g_\rho(s_1, s) := \langle v_1, v_2 \rangle_{L^2(d\rho)} = \int_{\mathbb{R}^d} v_1(x) \cdot v_2(x) \mathrm{d}\rho(x)$$

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- Wasserstein gradient $\mathrm{grad}_{\mathcal{W}} \mathcal{F}(\rho) \sim -\mathrm{div}(\rho\zeta)$? Chain rule $\mathcal{F} : \mathcal{P} \to \mathbb{R}$, curve ρ_t with tangent vector $s \sim -\mathrm{div}\, \rho v$ at $\rho_{t=0} = \rho$,

$$\frac{d}{dt} \mathcal{F}(\rho_t) \Big|_{t=0} = g_\rho(\mathrm{grad}_{\mathcal{W}} \mathcal{F}(\rho), s) = \int_{\mathbb{R}^d} \zeta(x) \cdot v(x) \mathrm{d}\rho(x)$$

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Formal rule :

$$\mathrm{grad}_{\mathcal{W}} \mathcal{F}(\rho) = -\mathrm{div} \left(\rho \nabla \frac{\delta \mathcal{F}}{\delta \rho} \right), \qquad \text{i.e. } \zeta = \nabla \frac{\delta \mathcal{F}}{\delta \rho}$$

Fundamental examples, $\mathrm{grad}_{\mathcal{W}} \mathcal{F}(\rho) = -\,\mathrm{div}\left(\rho \nabla \frac{\delta \mathcal{F}}{\delta \rho}\right)$

1. Internal energy $\mathrm{d}\rho(x) = \rho(x)\mathrm{d}x$

$$\mathcal{F}(\rho) = \int f(\rho(x))\mathrm{d}x \qquad \Rightarrow \qquad \mathrm{grad}_{\mathcal{W}} \mathcal{F}(\rho) = -\,\mathrm{div}(\rho \nabla f'(\rho))$$

- Heat equation $\partial_t \rho = \Delta \rho = \mathrm{div}(\rho \nabla \log(\rho))$, gradient flow $\partial_t \rho = -\,\mathrm{grad}_{\mathcal{W}} \mathcal{H}(\rho)$ of the Boltzmann entropy $\mathcal{H}(\rho) = \int \rho \log \rho$ [Jordan-Kinderlehrer-Otto, '98]
- Porous Media Equation $\partial_t \rho = \Delta \rho^m = \mathrm{div}\left(\rho \nabla \left(\frac{m}{m-1} \rho^{m-1}\right)\right)$, gradient flow $\partial_t \rho = -\,\mathrm{grad}_{\mathcal{W}} \mathcal{E}_m(\rho)$ of $\mathcal{E}_m(\rho) = \frac{1}{m-1} \int \rho^m$ [Otto, '99]

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2. Potential energy

$$\mathcal{F}(\rho) = \int V(x)\,\mathrm{d}\rho(x) \qquad \Rightarrow \qquad \mathrm{grad}_{\mathcal{W}}\mathcal{F}(\rho) = -\,\mathrm{div}(\rho\nabla V)$$

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3. Interaction energy

$$\mathcal{F}(\rho) = \frac{1}{2}\iint G(x-y)\mathrm{d}\rho(x)\mathrm{d}\rho(y) \qquad \Rightarrow \qquad \mathrm{grad}_{\mathcal{W}} \mathcal{F}(\rho) = -\,\mathrm{div}(\rho\nabla(G*\rho))$$

Back to PNP

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product space $z=(u,v)\in\mathcal{M}=\mathcal{P}\times\mathcal{P}$ and distance $d_z^2=\mathcal{W}_u^2+\mathcal{W}_v^2$

Gradient flow $\frac{dz}{dt}=-\operatorname{grad}_d\mathcal{E}(z)$

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$$\frac{1}{2}\int|\nabla\Psi|^2=\frac{1}{2}\int(-\Delta\Psi)\cdot\Psi=\frac{1}{2}\iint[u-v](x)G(x-y)[u-v](y)\,\mathrm{d}x\mathrm{d}y$$

Theorem [KMX '14]

Let $u^0, v^0 \in L^m \cap L^{2d/(d+1)} \cap \mathcal{P}^2(\mathbb{R}^d)$. Then there exists a global weak energy solution $u(t), v(t) \in \mathcal{C}^{1/2}([0,\infty); \mathcal{M} \cap W^{-s,r})$ such that

$$\forall\, 0 \le t_1 \le t_2 : \qquad \mathcal{E}(u(t_2), v(t_2)) \le \mathcal{E}(u(t_1), v(t_1)) \le \mathcal{E}(u^0, v^0) < \infty.$$

Moreover if $u^0, v^0 \in L^p(\mathbb{R}^d)$ for $p \in [1,\infty]$ then

$$\|u(t)\|_{L^p(\mathbb{R}^d)} + \|v(t)\|_{L^p(\mathbb{R}^d)} \le e^{\Lambda t}(\|u^0\|_{L^p(\mathbb{R}^d)} + \|v^0\|_{L^p(\mathbb{R}^d)})$$

with $\Lambda = \max\left\{\|\Delta U\|_{L^\infty(\mathbb{R}^d)}, \|\Delta U\|_{L^\infty(\mathbb{R}^d)}\right\}$.

Rmk1 : no uniqueness ? weak $\partial_t z = \mathrm{div}(J)$ with $J_u, J_v \in L^2_{loc}([0,\infty); L^1)$
Rmk2 : existence [Gajewski '94, Jüngel '97,Kurokiba-Ogawa '08] in bounded domains, higher gradient/regularity for initial data, linear diffusion (fixed points). No L^p control.
Formal long time asymptotics : entropy methods [Biler-Dolbeault-Markowich '99].

Abstract theory of gradient flow in metric spaces [Ambrosio-Gigli-Savaré ∼'08] : if the driving energy functional is λ-geodesically convex

$$\mathcal{E}(x_t) \leq (1-t)\mathcal{E}(x_0) + t\mathcal{E}(x_1) - \frac{\lambda}{2}t(1-t)d(x_0, x_1)$$

then abstract existence results, contractivity, uniqueness, long time convergence, etc...

Challenges

- Multicomponent + G, U, V non convex (multiple wells) : no λ-convexity (even locally)
- Singular kernel $G(x) = C_d/|x|^{d-2}$: delicate regularity issues
- Nonlocal long-range interaction $G(x) > 0$ in $\mathbb{R}^d$
- Nonlinear degenerate diffusion $\Delta\rho^m$: no smoothing

Strategy of proof

Smooth flows $\partial_t x = -D\mathcal{F}(x)$ in Hilbert spaces

$$\frac{x^{n+1} - x^n}{h} = -D\mathcal{F}(x^{n+1}) \quad \Leftrightarrow \quad x^{n+1} = \text{Argmin}\left(x \mapsto \frac{1}{2h}\|x - x^n\|_H^2 + \mathcal{F}(x)\right)$$

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DeGiorgi's minimizing movement

For fixed $h > 0$ and initial data $z^{(0)} = (u^0, v^0)$ with $\mathcal{E}(z^0) < \infty$, define

$$z^{(n+1)} \in \text{Argmin}\left(z \mapsto \frac{1}{2h} d^2(z, z^{(n)}) + \mathcal{E}(z)\right)$$

and the piecewise constant time interpolation

$$z_h(t) := z^{(n)}, \qquad t \in [nh, (n+1)h).$$

Retrieve the weak solution as $z(t) = \lim_{h \downarrow 0} z_h(t)$.

Purely variational ! Monotonicity $\mathcal{E}(z^{(n+1)}) \leq \mathcal{E}(z^{(n)}) \leq \mathcal{E}(z^0) < \infty$

Technical aspects

1. Minimization problem : lower semi-continuity and compactness of sublevelsets ? compatibility between $d_z^2 = \mathcal{W}_u^2 + \mathcal{W}_u^2$, $\mathcal{E}$, and intermediate topologie ?
2. Hardy-Littlewood-Sobolev inequalities $\Psi = G * (u - v)$
3. Euler-Lagrange equations ? Formal Riemanian calculus (Wasserstein non Euclidean), extra regularity for the minimizers. very technical, *flow interchange* technique [Matthes-McCann-Savaré, '09]
4. Compactness for $z_h(t) \to z(t)$: Aubin-Lions-Simon in space (energy monotonicity but only L^1) and time ($W^{-s,r}$ and metric setting). Nonlinear terms $\nabla u^m, \nabla v^m$ and $u\nabla\Psi, v\nabla\Psi$: strong convergence (a.e. (t,x))