Dynamics of adhesive particles and optimal transportation of mass

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Overview

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- Fragmentation and Coagulation

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- Zero-pressure gas dynamics and shock waves as models of coagulations

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  (I) Inner energy
  (II) Extended Lagrangian systems

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Density of clusters of size n is given by $f(n,t)$. The evolution equation:

$$\frac{\partial f(n,t)}{\partial t} = \int_0^n K_c(n-m,m) f(m,t) dm - f(n,t) \int_n^\infty K_c(n,m) dm + \int_0^\infty K_f(n+m,m) f(m+n,t) dm - f(n,t) \int_0^n K_f(n,m) dm \quad (1)$$

Consider a swarm of N particles of masses m_i whose orbits are given by $x_i(t)$. The initial (at $t = 0$) positions and velocities of the particles are prescribed

$$x_i(0) := x_i^{(0)} \quad ; \quad \dot{x}_i(0) = v_i^{(0)} \ .$$

If there are no external forces, then, at least until two (or more) particles collide, the orbits of the particles are given by

$$x_i(t) = x_i^{(0)} + t v_i^{(0)} \ .$$

In the limit

$$\rho(x, 0) = \lim_{N \to \infty} N^{-1} \sum^{N} m_i \delta_{x_i^{(0)}}$$

$$(\rho \vec{u})(x, 0) = \lim_{N \to \infty} N^{-1} \sum^{N} m_i v_i^{(0)} \delta_{x_i^{(0)}} \ ,$$

the density and velocity fields satisfies, formally, the system of conservation law (*zero-pressure dynamics*)

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho \vec{u}) = 0 \quad ; \quad \frac{\partial (\rho \vec{u})}{\partial t} + \nabla_x \cdot (\rho \vec{u} \otimes \vec{u}) = 0 \ .$$

This system can be viewed as an initial value problem, subjected to

$$\rho(x,0) = \rho_0(x) \geq 0 \quad , \quad \vec{u}(x,0) = \vec{u}_0(x) \ .$$

As long as the solution is *classical* (namely, continuously differentiable), the momentum equation can be written as the Burger's equation

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Zero pressure and dynamics of adhesive particles

- Zeldovich (1970): Sticky particle model.
- Existence: E, Rykov and Sinai (1996) Brenier and Grenier (1998), ect.
- Uniqueness: Bouchut and James (1999)

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- Hence, there are no fragmentation waves!
- The process of fragmentation is currently described by phenomenological kernels. It is based on ad hoc probabilistic assumptions which have nothing to do with the fundamental principle of physics!
- In physics, reversible processes are usually derived from an action principle.

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$$A(\vec{x}; T) := \int_0^T L\left(m_1 \dot{x}_1, \ldots m_N \dot{x}_N\right) dt$$

where

$$L(p_1, \ldots p_N) := \sum_1^N \frac{|p_i|^2}{2m_i}$$

and

$$\underline{A}(\vec{x}^{(0)}, \vec{x}^{(1)}; T) :=$$

$$\min_{\vec{x}(\cdot)} \left\{ A(\vec{x}; T) \; ; \; \vec{x}(0) = \vec{x}^{(0)} \; , \vec{x}(T) = \vec{x}^{(1)} \right\} \; .$$

Note that here the masses m_i of the particles are constants.

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In order to implement collisions into an action principle, we must introduce inner energy, and allow particles to exchange mass.

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c) If for $\tau \in (0,T)$ there exists a subset $I \subset \{1, \ldots N\}$ for which $x_i(\tau) = x_j(\tau) \equiv x$ for all $i, j \in I$ while $x_l(\tau) \neq x$ for $l \notin I$, then

$$\sum_{i \in I} m_i(t^-) = \sum_{i \in I} m_i(t^+) \ .$$

Inner energy

There is a function $\xi = \xi(m)$, called the inner energy of a particle of mass m, such that

$$\xi \in C(\mathbb{R}^+) \ \ , \ \xi(0) = 0, \ \ \forall m_1, m_2 > 0$$
$$\Longrightarrow \xi(m_1) + \xi(m_2) < \xi(m_1 + m_2) \ .$$

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The dynamics of this system is obtained by the action: $A : \Gamma \to \mathbb{R}$ defined for $\gamma := (x_1, m_1 \ldots x_N, m_M)$ by

$$A(\gamma; T) := \sum_1^N \int_0^T \left[\frac{1}{2} m_i(t) \, |\dot{x}_i|^2 - \xi(m_i(t)) \right] dt$$

Theorem

If γ is a minimizer of the action A within the set Γ subjected to the end conditions $\gamma(0) = \left(x_1^{(0)}, m_1^{(0)} \ldots x_N^{(0)}, m_N^{(0)}\right)$,
$\gamma(T) = \left(x_1^{(T)}, m_1^{(T)} \ldots x_N^{(T)}, m_N^{(T)}\right)$, *then γ preserves both the linear momentum*

$$\mathbf{P} := \sum_1^N m_i(t)\dot{x}_i(t)$$

and energy

$$\mathbf{E} := \frac{1}{2}\sum_1^N m_i(t)\left|\dot{x}_i(t)\right|^2 + \sum_1^N \xi(m_i(t)) \ .$$

Extended Lagrangian formulation

Assume that the distribution of particles at time t is given by a positive measure $\mu_{(t)}$ on Ω. We usually denote a trajectory of probability measures $\mu_{(t)}$, $0 \leq t \leq T$ by μ. We denote the set $\mathbf{H}_2[0, T]$ as all such trajectories for which

$$\|\mu\|_{2,T}^2 := \inf_{\vec{E}} \int_0^T \left| \frac{d\vec{E}_{(t)}}{d\mu_{(t)}} \right|^2 \mu_{(t)}(dx)dt < \infty$$

$$\frac{\partial \mu}{\partial t} + \nabla_x \cdot \vec{E}_{(t)} = 0$$

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in the sense of distributions. For a given pair of probability measures μ_0, μ_1, the extended action principle is defined by

$$\underline{A}(\mu_0, \mu_1) := \min_{\mu} \frac{1}{2} \|\mu\|_{2,T}^2$$

$$\mu_{(0)} = \mu_0, \; \mu_{(T)} = \mu_1 \; .$$

The minimization problem is a special case of McCann interpolation

$$\mu_{(t)} = \left[\frac{T-t}{T}\mathbf{Id} + \frac{t}{T}\mathbf{S}\right]_{\#}\mu_0$$

where $\mathbf{S}$ is the map which realizes the optimal transportation of μ_0 to μ_1 under quadratic cost:

$$\inf_{\mathbf{S}_{\#}\mu_0=\mu_1} \int_{\Omega} |x-\mathbf{S}(x)|^2 \mu_0(dx)$$

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In case of discrete measure (D) The "Graph orbit" Γ is a special case of admissible μ:

$$\mu = \sum_1^N m_i(t) \delta_{x_i(t)}$$

$$\inf_\Lambda \sum_1^N \sum_1^N \Lambda_{i,j} |x_i - y_j|^2 \ ,$$

where $\sum_i \Lambda_{i,j} = m_j(T)$, $\sum_j \Lambda_{i,j} = m_i(0)$.

Extended action subjected to a prescribed pressure

The extended Lagrangian with a pressure

$$A_P(\mu) = \frac{1}{2}\|\mu\|_2^2 - \int_0^T P(x,t)\mu_{(t)}(dx)dt \ .$$

The associated Hamilton-Jacobi equation

$$\frac{\partial \phi}{\partial t} + \frac{1}{2}|\nabla_x \phi|^2 + P = 0 \quad ; \quad (x,t) \in \Omega \times (0,T) \ ,$$

and the continuity equation

$$\frac{\partial \mu_{(t)}}{\partial t} + \nabla_x \cdot \left(\mu_{(t)} \nabla_x \phi\right) = 0 \ .$$

The end conditions:

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Theorem

For any pair of end conditions μ_0, μ_1 there exists an orbit $\mu \in \mathbf{H}_2([0,T])$ which realizes the infimum of A_P.

Some definitions

The cost function:

$$C_P(x,y,\tau,t) :=$$
$$\min\left\{\int_\tau^t \left(\frac{|\dot{\overline{x}}|^2}{2} + P(\overline{x}(s),s)\right) ds \quad ; \quad \overline{x}:[\tau,t]\to\Omega\right\} \quad (2)$$

where $\overline{x}(\tau)=y,\ \overline{x}(t)=x$.

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where $\overline{x}(\tau) = y$, $\overline{x}(t) = x$. In particular, if $P = 0$:

$$C_0(x, y, \tau, t) := \frac{|x - y|^2}{2(t - \tau)} \ .$$

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i) A forward (res. backward) solution is defined, for $t \in [0, T]$, by
$\overline{\phi}(x,t) := \min_y \{C_P(y,x,0,t) + \phi(y,0)\}$, res.
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iii) $(\overline{\phi}, \underline{\phi})$ is called a reversible pair if $\overline{\phi} = \underline{\phi}$ on Ω for $t = 0$ and $t = T$. In this case, $\overline{\phi}(x,t) \geq \underline{\phi}(x,t)$ on $\Omega \times [0,T]$.

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iv) If $(\overline{\phi}, \underline{\phi})$ is a reversible pair, then the reversibility set is defined by
$K_0(\overline{\phi}, \underline{\phi}) := \{(x,t) \in \Omega \times (0,T) \; ; \; \overline{\phi}(x,t) = \underline{\phi}(x,t) := \psi(x,t)\}$
$\nabla_x \psi(x,t) = \nabla_x \overline{\phi} = \nabla_x \underline{\phi}$ is Lipschitz on the reversibility set.
We call ψ a reversible solution.

Theorem

If ϕ_0, ϕ_1 *maximizes* $\int_\Omega (\phi_1\mu_1(dx) - \phi_0\mu_0(dx))$ *subjected* $\phi_1(x) - \phi_0(y) \leq C_P(x, y, 0, T)$ *for any* $x, y \in \Omega$, *then* $\{\phi_0, \phi_1\}$ *is a reversible pair. The reversibility function* ψ *verifies the Hamilton-Jacobi equation, and the optimal solution of* A_P *is supported in* $K_0(\phi_0, \phi_1)$ *and verifies the continuity equation subjected* $\nabla\phi = \nabla\psi$. *Moreover, the flow*

$$\frac{d\mathbf{S}^{(t,s)}}{dt} = \nabla\psi\left(\mathbf{S}^{(t)}_{(x)}, t\right) \quad ; \quad \mathbf{T}^{(t,t)} := \mathbf{I_d}$$

transports this orbit $\mathbf{S}^{(\mathbf{t},\mathbf{s})}_{\#}\mu_{(\mathbf{s})} = \mu_{(\mathbf{t})}$.

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- *The particles of the optimal flow subjected to a prescribed pressure do not collide (and, in particular, do not stick).*
- *There are no shock waves for the Hamilton-Jacobi equation. Indeed,* ψ *is a reversible solution, as claimed.*

Implementation of the Inner energy

We now wish to extend the action principle to orbits composed of (Borel) measures in Ω. Let $\overline{\mathcal{M}}$ be the set of such probability Borel measures. For any $\mu \in \overline{\mathcal{M}}$ set $\mu = \mu^{pp} + \tilde{\mu}$ to be its *unique* decomposition into its atomic and non-atomic parts. For each $\mu \in \overline{\mathcal{M}}$ we define the inner energy $\Xi(\mu)$ as

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For any $\mu \in \mathbf{H}_2([0, T])$ define the action as:

$$A_{\Xi}(\mu; T) := \frac{1}{2}\|\mu\|^2_{2,T} - \int_0^T \Xi(\mu_{(t)})dt \ .$$

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Remark: The assumption $\xi(m) = m^{\sigma}$ for $\sigma > 1$ verifies verifies this condition.

Lemma

The action $A_{\Xi}(\cdot, T)$ *is lower-semi-continues (l.s.c) with respect to* $C([0, T]; C^*(\Omega))$.

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Theorem

Given $\mu_0, \mu_1 \in \overline{\mathcal{M}}$, *there exists an action minimizer* $\mu \in \mathbf{H}_2[0,T]$ *for*

$$\underline{A}(\mu_0, \mu_1; T) := \min_{\mu} A_{\Xi}(\mu, T)$$

subjected to $\mu_{(0)} = \mu_0 \quad , \quad \mu_{(T)} = \mu_1$

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Let $J : \mathbb{R}^+ \to \mathbb{R}^+$ be a convex function satisfying $J(0) = J^{'}(0) = 0$. Let $\theta \in C_0^\infty(\Omega; \mathbb{R}^+)$ such that $\theta(0) = 1 \geq \theta(x)$ for all $x \in \Omega$. For each $\epsilon > 0$, the inner energy function ξ corresponding to J is defined by

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Lemma

For each $\epsilon > 0$, $\mu \to -\int_0^T \Xi_\epsilon\left(\mu_{(t)}\right) dt$ is continuous in the weak topology of $\mathbf{H}_2[0, T]$.

Let now

$$A^{\epsilon}_{\Xi}(\mu; T) = \frac{1}{2}\|\mu\|^2_{2,T} - \int_0^T \Xi_\epsilon\left(\mu_{(t)}\right) dt \ .$$

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Let μ_ϵ a minimizer of A^{ϵ}_{Ξ}. Since the set μ_ϵ, $0 < \epsilon < 1$, is pre-compact in $\mathbf{H}_2[0, T]$, we can look for a limit point of a subsequence of μ_ϵ as $\epsilon \to 0$

Consider now the pair of equations

$$\frac{\partial \mu}{\partial t} + \nabla \cdot (\mu \nabla_x \psi) = 0$$
$$\frac{\partial \psi}{\partial t} + \frac{1}{2} |\nabla_x \psi|^2 - P_\epsilon = 0 \ ,$$

where

$$P_\epsilon(x,t) = -\Xi_\epsilon'(\mu_{(t)})_{(x,t)} :=$$
$$\epsilon^{-1} \int_\Omega J' \left(\int_\Omega \theta_\epsilon(z-y) \mu_{(t)}(dz) \right) \theta_\epsilon(x-y) dy \ . \quad (3)$$

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Example

: if $\mu = \sum m_i \delta_{x_i}$ then

$$P_\epsilon(x,t) \approx J' \left(\sum_j m_j \theta \left(\frac{x_j - x}{\epsilon} \right) \right) \ .$$

Very strong and very short range repelling force!

Theorem

If $\overline{\mu}^{(\epsilon)}$ *is a maximizer of the action* $A^{\epsilon}_{\underline{=}}$ *then there exists a reversible-pair solution* $(\overline{\phi}^{(\epsilon)}, \underline{\phi})^{(\epsilon)}$ *The reversibility set* $K_0(\overline{\phi}^{(\epsilon)}, \underline{\phi}^{(\epsilon)})$ *contains the support of* $\overline{\mu}^{(\epsilon)}$ *in* $\Omega \times (0, T)$*. In addition, the reversibility set is invariant under the flow generated by the reversible solution*

$$\frac{d\mathbf{S}_{(\epsilon)}{}^{(s,t)}(x)}{dt} = \nabla \psi^{(\epsilon)} \left(\mathbf{S}^{(s,t)}_{(\epsilon)}(x), t \right) \ .$$

As $\epsilon \rightarrow 0$*, the particles' orbits* $\mathbf{S}^{(s,t)}_{(\epsilon)}$ *converge to a set-valued mapping* $\mathbf{S}^{(s,t)} : \Omega \rightarrow \mathcal{B}(\Omega)$ *so that* $\lim_{\epsilon \rightarrow 0} \mathbf{S}^{(s,t)}_{(\epsilon)}(x) \in \mathbf{S}^{(s,t)}(x)$.

Formal evolution equations in 1D

Suppose now an optimal transport is presented by the pair μ, ϕ where

$$\mu_{(t)}(dx) = \rho(x,t)dx + \sum m_i(t)\delta_{x_i(t)}dx \ ,$$
$$\int_\Omega \rho(x,t)dx + \sum m_i(t) = 1 \ . \quad (4)$$

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The continuity equation takes the form

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho \nabla_x \psi) + \sum \dot{m}_i(t)\delta_{x_i(t)} = 0 \ .$$

and the momentum equation

$$\frac{\partial \psi}{\partial t} + \frac{1}{2}|\nabla_x \psi|^2 + \sum \xi'(m_i(t))\,\mathbf{1}(x_i(t) - x) = 0 \ ,$$

where $\mathbf{1}(x) = 0$ if $x \neq 0$, $\mathbf{1}(1) = 1$.

Reversible solution in the limit $\epsilon = 0$

The limit action function

$$C(y, x, \tau, t; \mu) := \inf_{\overline{x}} \left\{ \int_\tau^t \left(\frac{1}{2}|\dot{\overline{x}}(s)|^2 - \sum_{\mu_{(s)}(\{x\})>0} \xi'(\mu_{(s)}(\{x\})) 1_{(\overline{x}(s),s)} \right) ds \right\}$$

where the infimum is taken on the set of orbits $\overline{x} : [\tau, t] \to \Omega$ satisfying $\overline{x}(\tau) = y$, $\overline{x}(t) = x$.

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Fragmentation:

$$\psi(x, t) = \inf_{y \in \Omega} [C(y, x, 0, t; \mu) + \phi_0(y)] \leq \overline{\phi}(x, t) := \inf_{y \in \Omega} \left[\frac{|x - y|^2}{2t} + \phi_0(y) \right] \tag{5}$$

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Coagulation:

$$\underline{\phi}(x, t) := \sup_{y\in\Omega} \left[-\frac{|x - y|^2}{2(T - t)} + \phi_1(y) \right] \le \sup_{y\in\Omega} [C(x, y, t, T; \mu) + \phi_1(y)] = \psi(x, t) \quad (6)$$

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$$\frac{|\alpha_i|^2(t)}{8} - \xi^{'}(m_i(t)) = 0 \ ,$$

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$$\text{Fragmentation} : \quad \frac{dm_i}{dt} = -\overline{\rho}_i(t)\sqrt{8\xi_i'(m_i)} \ , \ .$$

while the particle's orbit satisfies the Rankine-Hugoniot condition:

$$\dot{x}_i = \frac{1}{2}\left[\psi_x(x_i^+(t),t) + \psi_x(x_i^-(t),t)\right]$$
$$:= \frac{\partial}{\partial x}\psi_0(x_i(t),t) + \sum_{j\neq i}\alpha_j(t)\frac{x_i(t)-x_j(t)}{|x_i(t)-x_j(t)|}\ . \quad (7)$$

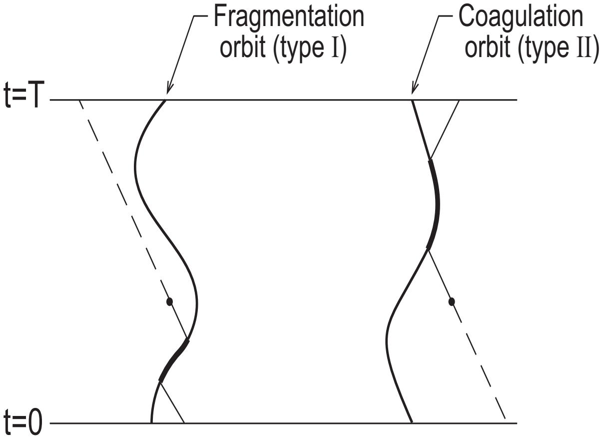

Figure: A representation of a reversible solution. Bold curves: particle orbits. Bold dots: observers positions at time t. Light curves: the characteristic curves for forward (res. backward) solution in the vicinity of type (I) (res. type (II)) orbit. Dashed light lines: the characteristic curves for forward (res. backward) solution in the vicinity of type (II) (res. type (I)) orbit.

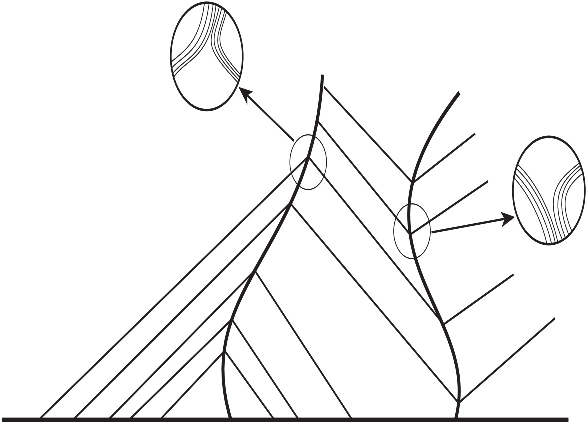

Figure: Same as in Fig. **??**, where the relaxation is emphasized in the magnifying lens.