Hard Spheres Dynamics:

estimating the collisions through Compensated Integrability

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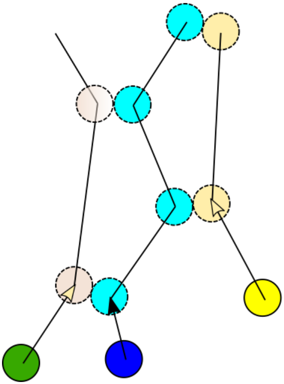
A simple model

- Open space $\mathbb{R}^n$. *No boundary, no periodicity.*
- A large but finite number N of spherical bodies of equal radii a and masses m.
  Think to $N \sim 10^{23}$ (Avogadro).
- Neither external forces, nor short/long-range interaction.
- Only Elastic collisions.
  Between collisions, every particle travels with constant velocity.



Pairwise collisions

Two particles centered at X_1, X_2. Incoming velocities v_1, v_2, outgoing velocities v_1', v_2'. At the collision time

$$\|X_2 - X_1\| = 2a.$$

Conservation of momentum/energy

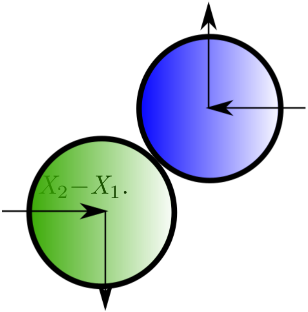
$$\begin{aligned} v_1' + v_2' &= v_1 + v_2, \\ \|v_1'\|^2 + \|v_2'\|^2 &= \|v_1\|^2 + \|v_2\|^2. \end{aligned}$$

Friction-less collisions

Define $[v_1] := v_1' - v_1 [v_1] = -[v_2] [v_1] \quad \| \quad X_2 - X_1.$

These define a smooth map

$$(v_1, v_2) \longmapsto (v_1', v_2').$$



Drawn in the moving frame attached to the center of mass.

The Cauchy problem

Initial positions/velocities $X_i(0)$ and $v_i(0)$ $(i = 1, \dots N)$ are given.

The dynamics is well-defined as long as

- no particle collides with more than one other at a time,
- collisions do not accumulate.

Theorem 1 (R. K. Alexander, 1975.)

For generic initial data, the Cauchy problem admits a unique, global-in-time solution, with only pairwise collisions, forming a discrete set.

Sinaï's Problem : Is the collision set finite ?

In other words : $\exists ?$ a time T^*, after which there are not any more collisions ?

> *YES : L. N. Vaserstein (1979), R. Illner (simpler proof, 1989/90). They do not estimate the number of collisions.*

Bounds.

$$\#\{\text{collisions}\} \leq \left(32N^{3/2}\right)^{N^2} \qquad \text{(Burago \& al., 1998).}$$

$$\#\{\text{collisions}\} \quad \text{can be} \geq \begin{cases} \frac{1}{27}\,N^3 & \text{(Burdzy \& Duarte, 2018),} \\ 2^{\lfloor \frac{N}{2} \rfloor} \quad (n \geq 3), & \text{(Burago \& Ivanov, 2019).} \end{cases}$$

Burago & Ivanov's claim

> *It seems that, if the number of collisions is "large", then the overwhelming number of collisions are "inessential" in the sense that they result in almost zero exchange of momenta, energy, and directions of velocities of balls.*
>
> *We will think about it tomorrow*[1].

Could be important when passing to the thermodynamic limit $N \to +\infty$. Inessential collisions do not contribute to the macroscopic pressure, nor to the stress tensor.

1. Borrowed from *Gone with the wind.*

B. & I.'s claim is TRUE !

Theorem 2 (D. S., 2019)

Denote $\mathbf{v}$ *the standard deviation of the velocities (a conserved quantity). Then*

$$\sum_{\text{coll.}} \|v' - v\| \leq c_n N^2 \mathbf{v}.$$

In addition,

$$\sum_{\text{coll.}} \|v \times v'\| \leq c_n N^2 \mathbf{v}\, \bar{v},$$

where $\bar{v}$ *denotes the quadratic mean velocity.*

Interpretations

- Each particle experiences (in average) an $O(N)$ number of essential collisions. By essential, we mean $\|v' - v\| \sim \mathbf{v}$.

  The inessential collisions satisfy $\|v' - v\| \ll \mathbf{v}$.
- Averaging over the particles, the momentum $q_\alpha := mv_\alpha$ satisfies

$$\langle\, TV(t \mapsto q_\alpha(t))\,\rangle \leq 2c_n M\mathbf{v} \leq 2c_n\sqrt{2ME}$$

  where M is the *total mass* and E the *total energy*.

Mesoscopic models (Boltzman, ...) should be consistent with these conclusions.

Outline of the proof

1. Build a divergence-free positive semi-definite tensor encoding the dynamics.
   - Mimics the tensor $\begin{pmatrix} \rho & \rho v \\ \rho v & \rho v \otimes v + pI_n \end{pmatrix}$ of gas dynamics, whose row-wise divergence vanishes (Euler equations).
   - We look for a discrete analogue : our tensor is singular (supported by a graph).
2. Complete this tensor by adding a parametrized corrector at each node of the graph, so as it be "positive definite".
3. Apply a *modified version* of <u>Compensated Integrability</u>, taylored for graph-supported tensors.
4. Adjust the parameters to optimize the functional inequality.

Singular tensors

Consider a singular vector field over $\mathbb{R}^d$,

$$V = u\,\mathcal{L}_{(a,b)}, \qquad u \in \mathbb{R}^d,$$

where $\mathcal{L}_I$ is the Lebesgue measure along an interval I.

$$\langle V, \vec{\theta}\rangle = \int_a^b u \cdot \vec{\theta}\, d\mathcal{L} = \int_0^\ell u \cdot \vec{\theta}(a + s\frac{b-a}{|b-a|})\, ds.$$

Assume that u is parallel to $b - a$ (say pointing in the same direction).

Then

$$\begin{aligned}\langle \operatorname{div} V, \phi\rangle &= -\langle V, \nabla\phi\rangle = -\int_0^\ell u\cdot\nabla\phi(a+s\frac{u}{|u|})\,ds \\ &= |u|(\phi(a)-\phi(b)).\end{aligned}$$

Hence

$$\operatorname{div} V = |u|(\delta_a - \delta_b).$$

Let us consider a tensor instead (symmetric, positive semi-definite)

$$S = \frac{u}{|u|}\otimes V = \frac{u\otimes u}{|u|}\,\mathcal{L}_{(a,b)}.$$

The row-wise Divergence satisfies

$$\operatorname{Div} S = u(\delta_a - \delta_b).$$

It is not divergence-free, though only because of the vertices a and b.

But :

Proposition 1

Let $a, b_1, \dots, b_r$ be given points and $u_j \parallel b_j - a$. Define

$$S = \sum_j \frac{u_j \otimes u_j}{|u_j|} \mathcal{L}_{(a,b_j)}.$$

Then $\mathrm{Div}\, S$ does not charge a, IFF (Kirchhoff's law)

$$\sum_j u_j = 0.$$

The mass-momentum tensor (I)

Consider a global-in-time dynamics of N hard spheres in $\mathbb{R}^n$. Set

$$d = 1 + n.$$

Independent variables are $(t, x) \in \mathbb{R}^d$.

The center of the j-th particle has velocity $v_j(t)$, piecewise constant. Form

$$u_j = \begin{pmatrix} 1 \\ v_j \end{pmatrix} : \mathbb{R} \to \mathbb{R}^d.$$

Denote $\gamma_j \subset \mathbb{R}^d$ the graph of the trajectory ; a broken line with nodes $Y_{j,m}$.

First attempt

Define

$$S^j = \frac{u_j \otimes u_j}{|u_j|} \mathcal{L}_{\gamma_j} \,,$$

then

$$S := \sum_{j=1}^{N} S^j .$$

One has

$$\mathrm{Div}_{t,x} S^j = \sum_m \begin{pmatrix} 0 \\ [v_j] \end{pmatrix} \delta_{Y_{j,m}}, \qquad [v_j] := v_j' - v_j \,.$$

The points $Y_{j,m}$ are pairwise distinct – centers remain distant at collisions ($2a$ apart) : S is <u>not</u> Divergence-free (Dirac masses do not cancel each other when summing over j).

The mass-momentum tensor (II)

Cancellation occurs when introducing virtual particles :

Collitons

Let a collision involve the i-th and j-th particles at time τ. Corresponding nodes at Y_i and $Y_j \in \mathbb{R}^d$, define

$$Q = \begin{pmatrix} 0 \\ q \end{pmatrix}, \qquad q = [v_i] = -[v_j],$$

then set

$$C = \frac{Q \otimes Q}{|Q|} \mathcal{L}_{(Y_i, Y_j)}.$$

We have as before

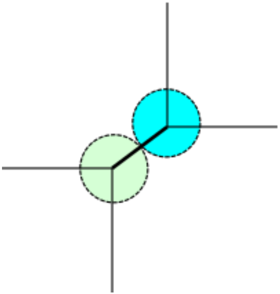
$$\mathrm{Div}_{t,x} C = Q(\delta_{Y_j} - \delta_{Y_i}).$$

This suggests to define the mass-momentum tensor of the configuration as

$$M = S + \sum \text{collitons.}$$

Theorem 3

The mass-momentum tensor M is symmetric, positive semi-definite and Divergence-free.



Detail of the support of the m.-m. tensor (projection over $\mathbb{R}^n_x$). The bold segment supports a colliton.

Rk. $\mathrm{Div}_{t,x} M \equiv 0$ encodes the conservation of mass ($=$ cons. of particles) and of momentum. It tells nothing about the kinetic energy.

Compensated Integrability

A Functional Analysis tool, reminiscent to the embedding

$$W^{1,1}(\mathbb{R}^d) \subset L^{\frac{d}{d-1}}(\mathbb{R}^d).$$

Theorem 4 (D. S., 2018-19)

Let A be a $d \times d$ tensor over $\mathbb{R}^d$, whose entries a_{pq} are finite measures. Assume that A is symmetric, positive semi-definite : for every $\xi \in \mathbb{R}^d$, the finite measure $\xi^T A \xi$ is non-negative.
Assume that the coordinates of the vector field $\mathrm{Div}\, A$ are finite measures.

Then the finite measure $(\det A)^{\frac{1}{d}}$ is actually a function, of class $L^{\frac{d}{d-1}}$. One has

$$\left\| (\det A)^{\frac{1}{d}} \right\|_{\frac{d}{d-1}} \leq c_d \|\mathrm{Div}\, A\|_{\mathcal{M}}. \tag{1}$$

Theorem 4 does not apply directly to the m.-m. tensor M :

- Its entries are only locally finite measures, because they extend to infinity. *Cure : truncation.*
- Estimate (1) is trivial because both sides vanish :
  - M is Divergence-free, (*no more after truncation*)
  - $(\det M)^{\frac{1}{d}} \equiv 0$, since the rank is either $0, 1$ or 2 while $d \geq 3$. *Cure : add correctors at the nodes.*
- Even after correction, $\widetilde{M}$ charges only segments, where it is rank-1. Still : $(\det \widetilde{M})^{\frac{1}{d}} \equiv 0$.

Determinantal masses

Heuristic example. $d = 2$ ($n = 1$). Consider the simplest case

$$M = \begin{pmatrix} \mathcal{L}_1 & 0 \\ 0 & \mathcal{L}_2 \end{pmatrix}$$

where $\mathcal{L}_j$ is the Lebesgue measure over the j-th axis. It is true that $(\det M)^{\frac{1}{2}} \equiv 0$. But $\det M$ makes sense in $\mathcal{D}'$ and is $\neq 0$ because

$$\mathcal{L}_1 \cdot \mathcal{L}_2 = \delta_{x=0}.$$

This suggests that for $d \geq 3$, m.-m. tensors satisfy

$$\left(\det \widetilde{M}\right)^{\frac{1}{d-1}} \sim \delta_Y$$

at each node up to a weight : a determinantal mass.

Rk. At a node, $\widetilde{M}$ (truncated m.-m. plus correctors) is a positively homogeneous distribution, of degree $1-d$.

Theorem 5 (Pogorelov, 1978.)

There exists a convex function θ, positively homogeneous of degree 1 about Y, such that

$$\widehat{\mathrm{D}^2\theta} = \widetilde{M}.$$

If θ was a smooth function, we should have

$$\left(\det \widehat{\mathrm{D}^2\theta}\right)^{\frac{1}{d-1}} = \det \mathrm{D}^2\theta = \mathrm{Jac}(\nabla\theta)$$

and thus

$$\int_\Omega \left(\det \widetilde{M}\right)^{\frac{1}{d-1}} dx\, dt = \mathrm{vol}(\nabla\theta(\Omega)).$$

When θ is homogeneous of degree 1 (hence not smooth),

- the image of $\nabla\theta$ (homogeneous of degree 0) surrounds a convex body D,
  Rk. D solves *Minkowski's problem.*
- $\det \mathrm{D}^2\theta$ concentrates at the tip.

We identify $\left(\det \widetilde{M}\right)^{\frac{1}{d-1}}$ with $\mathrm{vol}(D)\,\delta_Y$.

Example : in dimension d,

$$(\mathcal{L}_1 \cdots \mathcal{L}_d)^{\frac{1}{d-1}} = \delta_{x=0} \qquad !$$

Definition 1

The determinantal mass of $\widetilde{M}$ at the node Y is

$$\mathrm{Dm}(\widetilde{M}; Y) = \mathrm{vol}(D).$$

The main theoretical result is that Compensated Integrability is valid when including the determinantal masses :

Theorem 6

With the assumptions of Theorem 4, the following Functional Inequality holds true,

$$\int_{\mathbb{R}^d} (\det A)^{\frac{1}{d-1}}\, dy + \sum_{\text{nodes}} \mathrm{Dm}(A; Y_j) \le c_d \|\mathrm{Div}\, A\|_{\mathcal{M}}^{\frac{d}{d-1}}. \tag{2}$$

Open problems

- Adapt the analysis to a bounded domain / torus.
- Build a divergence-free, semi-definite positive mass-momentum tensor when the (identical) shape of particles is not spherical.
- When particles interact through a radial, repulsive force, such a M.-M. tensor is available, though the collitons are replaced by *interactons*, supported by ruled surfaces. Exploit this structure in a way similar to that above.
- With a Lennard–Jones potential, the force is repulsive at short distance (good), but attractive at large ones (bad). What can be done ?
- What does Theorem 2 tell us about thermodynamic limit ?

Happy Birthday, Costas ! !