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OBSERVER INDEPENDENCE AND MOLECULAR FLOW

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ABSTRACT. Opinions and assertions are quoted and ventilated, sometimes validated, on the title topics.

As a contribution to the rite of my admittance to the *Accademia Peloritana dei Pericolanti*, I thought fitting to periclitate via my choice of the subject for this talk and via my obligation to report here how I figure out the solution of some attendant problems.

A controversy, made explicit in a sequence of carping papers by distinguished scientists, was occasioned by a dilemma met in gas dynamics as a model of molecular flows: an important inference was confirmed valid by experiments even though dictates of observer independence were disregarded in the proof. Then ground axioms of the theory of continua were declared bogus; mainly, it seems to me, not for their intrinsic content, but only because one axiom, largely tacit but of essence, called for the everlasting existence of material elements (a property not valid for gasses, surely). It is that axiom, when intertwined with the principle of objectivity (as, for a period, it was called), which may lead, by the way of certain deductions, to an incongruity. Thus the latter principle was put in doubt, and declared acceptable at most as a matter of convenience within restricted proofs.

Evidently it was ignored that the principle had a very great ancient progenitor. Epicurus himself, as explicit proposer of a view of nature based on events variously generated by the incessant motion of basic particles, the atoms, in a vacuum. As a Roman epigone of Epicurus, Lucretius, put in his celebrated *De Rerum Natura*:

> *. . . omnis, ut est igitur per se, natura duabus*
> *constitit in rebus; nam corpora sunt et inane,*
> *haec in quo sita sunt et qua diversa moventur.*[1]
>
> . . . all nature then, as it is of itself, is matter and void, built of these two things: for there are bodies and the void, in which they are placed and where they move hither and thither.[2]

[1] *T. Lucreti Cari De Rerum Natura. Libri Sex*. Edited with Introduction and Commentary by W. E. Leonard and S. B. Smith. The University of Wisconsin Press, 1930. I.419-421.

[2] *Lucretius on the Nature of Things*. Translated by Cyril Bailey. Oxford at the Clarendon Press, first published 1910; pp. 40-41.

When once I read those lines at a meeting of the Society of Natural Philosophy, Walter Noll exploded from the audience: “Vacuum is a vacuous concept!”, an Aristotelian cry vouching for a doctrine shared by many sages in the middle ages but exploded by humanists. The latter searched and finally found a copy of Lucretius’ book, believed lost; by its circulation they generated what historians of science deemed to be a cultural ‘swerve’ opening to the ‘frenzy’ of renaissance. The decisive remark in that book proclaims:

> Wherefore, however long you hang back with much objection, you must needs confess at last that there is void in things.[3]

Mercyfully, one may say that Noll had in mind a static monophasic body, for the whole ‘natura’ (as in one of his celebrated papers, where ‘body’ is modelled, as in the theory of continua, by a compact set); whereas motion and boundary of bodies involve necessarily an environment, either an alternative phase or an ‘inane’. As for the latter, physicists say: ‘inane’ (at least when the hotly disputed quantum vacuum is excluded) is the abode of fields of manifold nature. Even narrowing our interests to strictly mechanical scrutiny, void is the abode of the field of gravity. Under most circumstances an engineer has in mind that field is almost trivial, imposing one preferred oriented direction only. At the opposite extreme, it summons the General Theory of Relativity.

But let me return to my main concern for involving here Epicurus (Samos 341 – Athens 270 BCE). Of his immense opus, about 300 titles, only three letters and a few fragments have survived. The three letters are to friends and students at his school ‘The Garden’: to Herodotus (on Physics), to Pytholes (on Phenomena in the Sky), and to Menoeceus (on Happiness). The last one is the most favourite, but our concern here is for the first. Atomic theory is the subject of the letter, but what engrossed me in it was a repeated warning not to let preconceptions or dubious ways of examining and describing reality prevail. Within one of those admonitions (one that some scholars thought of as only incidental and uselessly repetitive) the explicit recommendation enticed me that we now call frame indifference be assured.

> τὸ δὲ ψεῦδος καὶ τὸ διημαρτημένον ἐν τῷ προσδοξαζομένῳ ἀεί ἐστιν <ἐπὶ τοῦ προσμένοντος> ἐπιμαρτυρηθήσεσθαι ἢ μὴ ἀντιμαρτυρηθήσεσθαι, εἶτ’ οὐκ ἐπιμαρτυρουμένου <ἢ ἀντιμαρτυρουμένου> [κατά τινα κίνησιν ἐν ἡμῖν αὐτοῖς συνημμένην τῇ φανταστικῇ ἐπιβολῇ, διάληψιν δὲ ἔχουσαν, καθ΄ ἣν τὸ ψεῦδος γίνεται.] [4]
>
> Falsehood and error always depend upon the intrusion of opinion <when a fact awaits> confirmation or the absence of contradiction, which fact is afterwards frequently not confirmed <or even contradicted> [following a certain movement in ourselves connected with, but distinct from, the mental picture presented – which is the cause of error.][5]

... consequent to the onset of an own motion; note the qualifier τινα, hinting of an acceleration. Perhaps you judge as preconceived my reading of Epicurus, particularly my final

[3] *Ibid.*, p. 40.

[4] *Diogenes Laertius. Lives of Eminent Philosophers*. Translated by R. D. Hicks.The Loeb Classical Library. 1925. Vol. II, p. 580.

[5] *Ibid.*, p. 581.

insistence on possibly disturbing effects of observer motion. However, it is stunning that scholars in continuum mechanics argued hotly, at the end of the 1900 on a rule settled clearly 300 years BCE. It could be called 'Rule of Epicurus' and accepted as incontestable. Actually, dud consequences of frame indifference are met when that rule is cojoined with the castigated axiom of permanence of material elements. Before dropping our pursuits in desperation, the footing of which permanence is asserted need be pondered carefully. Pasquale Giovine and I have already sweated over that chore and described the outcome. So, I may simply quote it for you [6]:

> In recent years, some papers were published with the aim of formulating a dynamics of continua for which the largely tacit primal axiom of absolute persistence of material elements fails. The glaring instance of such a body is a gas though the occasional placing of its dynamics within a course of lectures as a chapter of standard continuum mechanics seems to imply the opposite. We quote for all from Truesdell and Muncaster, page 3: "The kinetic gas ...is a continuous medium ...Not only is the kinetic theory a field theory, but also the kinetic gas is endowed with the very same field descriptors as continuum mechanics ..." and in a footnote ..."For an elementary introduction to the basic concepts and assumptions of continuum mechanics the reader may consult the book of C. Truesdell, A First Course in rational Mechanics ...". There, the mentioned primal axiom is glossed over (page 36) by a seemingly innocent Axiom of Impenetrability: "In continuum mechanics, contrarily, the mappings $\chi(\cdot,t) : \mathscr{B} \to \chi_\Omega(\mathscr{B},t)$ is assumed bijective, ..."

The further glaring omission in this text is the remark that the Axiom of Impenetrability is a far from innocent constraint on the theory as described up to that point, and consequently it calls for the introduction of reactions. Assuming that impenetrability occurs without demand for power, one may seek to obtain pure evolution equations from which reactions are eliminated but at some other costs, as we will show below. The identification of the latter costs is (and I steal here a term from the title of a paper by a colleague) a serendipitous contribution to continuum mechanics. In fact, it may perhaps even call for some amendment in the major contribution just quoted: it may possibly also have a bearing on some issue in molecular dynamics. I am aware that I now navigate in more perilous waters than those between Scylla and Charibdis. Still the danger I am in is far inferior than that faced by Galileo when, the evening before the close of the process, he was threatened to be accused of heresy, a lethal sin, if the next day he did not repudiate his assertion that the earth moves around the sun. Proof of guilt be his statement, in his book entitled *Discorsi e dimostrazioni matematiche intorno a due nuove scienze*, that (if you allow me to use today's parlance) material elements have perennial existence. Such statement gainsays the miracle of transubstantiation, a christian dogma. The extract below is from the introduction of the book in the first edition:

> *...tuttavia io pure il dirò affermando, che astraendo tutte l'imperfezzioni della Materia, e supponendola perfettissima, ed inalterabile, e da ogni*

[6] G. Capriz and P. Giovine (2018). "Classes of ephemeral continua". *Mathematical Methods in the Applied Sciences* **41**(3), 1175-1196. DOI: 10.1002/mma.4658; p. 1175.

> *accidental mutazione esente, tuttavia il solo esser materiale fà, che la machina maggiore fabbricata dell'istessa materia, e con l'istesse proporzioni, che la minore, in tutte l'altre condizioni risponderà con giusta simmetria alla minore, fuor che nella robustezza, e resistenza contro alle violente invasioni: mà quanto più sarà grande tanto à proporzione sarà più debole. E perche io suppongo la materia essere inalterabile, cioè sempre l'istessa, è manifesto, che di lei, come di affezzione eterna, e necessaria, si possano produr dimostrazioni non meno dell'altre schiette, e pure Matematiche.*[7]

Anyway to survive, I must ask for your forbearance. I must sketch first a theory which works without the axiom of impenetrability. Then introduce the axiom as a perfect constraint and show the result: apparently the so-called Cauchy's stress is the sum of two tensors, one accounting for the intimate exertions at a scale lower than gross, and the second for the exertions from the environment.

As already mentioned I have provided a model of bodies where the axiom of persistence fails and have proposed to call that model 'ephemeral' continuum. Colleagues have helped me to check, correct and expand my assertions, sometimes rushed. I will try to give you a hasty look at essential steps, using excerpts from our papers. Necessarily the ensuing theory is local in essence, and the image one envisages is of physical space divided into small cubic boxes, as broached in molecular dynamics, representative volume elements (r.v.e.) or *'loculi'*, of edge δ; each box is envisioned as inhabited at each instant by a multitude of sundry molecules so numerous and moving so randomly and possibly in and out of the loculus to be treated, in all, as a grand canonical ensemble.

Then, it was proposed to substitute, within the circumstances, the trajectories of the missing material elements with wind streak lines obtained, by integration, from the wind velocity $v(\tau,x)$ filtered over a loculus $\mathfrak{c}(x)$ (which is portrayed in its own separate space $\mathscr{E}_x$), whose mass center x is in a region $\mathscr{B}_\tau$ of the three-dimensional Euclidean space $\mathscr{E}$ occupied by the body at a time τ. A sharp view is presumed to allow us to distinguish sub–places y within $\mathfrak{c}(x)$. We may then imagine further that, by an even sharper view, we could explore a neighborhood of each y, as one does in standard kinetic theory, but now at one remove down. That exploration should let us measure the *velocity* w of each molecule in each neighborhood. Remark that, as in the kinetic theory but now within the neighborhood of y, we disregard knowledge of the sub–place of each molecule, but keep note of its velocity w.

The field of filtered wind velocity $v(\tau,x)$ leads directly to the field of its gradient $L(\tau,x)$ and, from the latter, one can obtain, by integration along the wind streak lines a fictitious *placement gradient* $F(\tau,x)$ via the equality

$$\dot{F} = LF;$$

the time-derivatives appearing above and below are meant to be evaluated along the wind streak-lines obtained artificially by formal integration of the equation

$$\frac{dx}{d\tau} = v(\tau,x).$$

[7] Galileo Galilei, *Discorsi e Dimostrazioni Matematiche intorno à due nuoue Scienze Attenenti alla Mecanica & i Movimenti Locali*. In Leida: appresso gli Elsevirii, 1638. *Giornata Prima*, p. 3.

But the introduction, in analogy with L, of a tensor B characterizing an affine motion best fitting locally the disorderly peculiar motion of molecules offers the opportunity of portraying local vicissitudes better than F. In particular the *suffusion*

$$\sigma := \mathrm{tr}(L-B)$$

puts in evidence, when multiplied by ρ, the instantaneous rate of mass change in the invented wind element. Moreover, when pursuing analogies with the standard theory, we could introduce a *mesoscopic displacement gradient* as a double vector G by using a differential equation which includes the effects of mass gain and loss

$$\dot{G} = BG - \frac{1}{2}\sigma G.$$

The best fit mentioned above as to the prerogative of B is based on the notion of two mesoscopic tensors (per unit mass): the *Euler's tensor of inertia* Y and the *tensor moment of momentum* K. They are bound together as in the theories of quasi-rigid bodies

$$K = YB^T,$$

thus it is B that descends from Y and K and satisfies the (usually named) balance of moment of inertia

$$\frac{\partial Y}{\partial \tau} + (\mathrm{grad}Y)\nu = BY - YB^T.$$

A third tensor has an essential role in the theory: the symmetric positive semi-definite Reynolds's tensor H. We quote only the set of equations on which the theory rests: balance of mass, of momentum, of moment of momentum, of Reynolds' tensor;

: – conservation of mass:

$$\frac{\partial \rho}{\partial \tau} + \mathrm{div}\,(\rho v) = \sigma\rho;$$

: – balance of momentum:

$$\rho\left[\frac{\partial v}{\partial \tau} + (\mathrm{grad}\ v)\, v + \frac{1}{2}\sigma v\right] = \rho b + \mathrm{div}\ T;$$

: – balance of moment of momentum:

$$\rho\left[\frac{\partial K}{\partial \tau} + (\mathrm{grad}\ K)v - BK - KB^T + \sigma K - H\right] = \rho O - A + \mathrm{div}\ \mathbf{m},$$

or,

$$\rho\left\{Y\left[\frac{\partial B}{\partial \tau} + (\mathrm{grad}\ B)v\right]^T - H\right\} = \rho O - A + \mathrm{div}\ \mathbf{m};$$

: – balance of agitation:

$$\rho\left[\frac{\partial H}{\partial \tau} + (\mathrm{grad}\ H)v + \sigma H\right] = \rho J - Z + \mathrm{div}\mathbf{j}.$$

Again the time-derivatives appearing above are meant to be evaluated along the wind streaklines obtained artificially by formal integration of the equation for $v(\tau)$, but the complex expressions of the left-hand sides are consequences of the double kinetic circumstances envisaged.

The set of equations above was judged by many as too complex as a response to the apparently simple demand as to how to proceed when the axiom of impenetrability fails to apply. In effect there is, in the set, a maze of details that need prudent and alert mathematical analysis. However, those details apart, the set is, formally, akin to that already accepted for quasi-rigid bodies. The equation for H, absent then, could even here be substituted by an improved version of the standard theorem of kinetic energy usually derived from the first three equations alone. I refrain from entering details here.

Closing my talk, I mention only two outcomes of my address: the already announced possible consequences on some essential steps in molecular dynamics; plus three figures, courtesy of Dr. Ceravolo, which illustrate solutions of our equations describing some granular flows.

To achieve the first outcome I return to the full complex system of equations but introduce wisely chosen constraints reducing the number of fields ultimately relevant and explore if the constraints might be perfect, *i.e.*, calling only for powerless reactions. The most conspicuous example is one requiring wind streak lines to coincide with particle paths: $G = F$ or $B = L$, for which the suffusion σ is always null. Although seeming to flout the key grounds for introducing the full theory, the constraint preserves, nevertheless, some distinguishing features. Following the traditional approach to dealing with constraints, we suppose that all compulsions be sums of an active term specified by a constitutive rule and a reactive term. The set of the latter being collectively such as to lead to a vanishing power for all strainings permitted by the constraint. The resulting system of pure balance equations is now:

$$
\begin{aligned}
&\frac{\partial \rho}{\partial \tau} + \operatorname{div}(\rho v) = 0, \\
&\rho\left(\frac{\partial v}{\partial \tau} + L v\right) + \operatorname{div}\left\{\rho\left[H - \left(\frac{\partial L}{\partial \tau} + (\operatorname{grad} L) v\right) Y\right]\right\} = \\
&\qquad = \rho b - \operatorname{div}\left(\rho O^T\right) + \operatorname{div}\left[\operatorname{sym}(T_a + A_a) - (\operatorname{div}\mathbf{m}_a)^T\right], \\
&\rho\left[\frac{\partial H}{\partial \tau} + (\operatorname{grad} H)\, v\right] = \rho J.
\end{aligned}
$$

Our attention is focused on the second equation and, in it, on the tensor $T + A$ appearing under the operator of divergence in the right-hand side. Recall that T was introduced, in the equation of Cauchy, to express in the end macro surface effects, whereas A was expressing volume effects, at the mesolevel, in the equation for moments. Thus T describes compulsions from the environment, whereas A describes intimate compulsions; they act now, finally, as a sum together and A might even prevail: the constraint forces them to act in unison. It is my opinion that, in molecular dynamics, one evaluates, numerically via computer, A rather than T and that even the celebrated Herleitung of Noll might require some revision.

Passing now to the second outcome, I copy the results of a radically different approach, where wind trajectories are abandoned to evidence gross effects. A new kinematics is based using supposed trajectories obtained by mixing wind velocity with collision effects. A terse rendition of H is based on its being symmetric semi-definite, so that it can be written in terms of eigenvalues χ_s^2, with $|\chi_s| = 1$, and unit eigenvectors h_s (s = 1, 2, 3)

$$H = \sum_{s=1}^{3} \chi_s^2 \, h_s \otimes h_s.$$

Thus, of H could be given the following sketch: it can be regarded as generated by the balanced and unhindered cross-flow of six countervailing and equally populous clusters of molecules with velocities $((\sqrt{2})^{-1}\chi_s \, h_s)$ and $(-(\sqrt{2})^{-1}\chi_s \, h_s)$ (s = 1, 2, 3) with χ_s non-negative square root of χ_s^2. Such metaphor justifies the attribution to H the meaning of a measure of balanced cross-over rate. Alternatively one could imagine the same sums counting the number of bounces due to collisions.

For simplicity and to make those events more evident, we consider below only stationary flows where the only fields involved are those of v and H and balanced and unhindered cross-over of molecules is prominently influential. The reasoning is purely kinetic; the laws of interaction are simply assumed to provide the balances. Then certain paths wholly separate from wind streaks (paths which we call ‘bundle streaks’) seem to describe incidents more vividly. In general, contrary to what happens for wind streaks, more than one such streak goes through each place within the body evidencing cross-flow. The picture we intend to draw issues from imagining the set of molecules transiting across each place partitioned into six bundles each one characterized by its own peculiar velocity. The latter is defined via the filtered velocity v and the spectral version of the tensor H:

$$\frac{1}{2}\left[\left(\sum_{i=1}^{3} \chi_i\right)^{-1} \chi_s\right] v \pm \left(\frac{1}{\sqrt{2}}\,\chi_s\right) h_s, \quad s = 1,2,3.$$

The six sets of paths are obtained by a process akin to that pursued in the definition of wind streaks, relying now on the six vector fields.

We refrain from pursuing here the consequences in general nor do we enter into details. We simply show three figures of plane flows with v in the plane, only one non-vanishing eigenvalue χ of H and the corresponding eigenvector h again in the plane with perfect bouncing only on the constraining planes. The first picture portrays a channel plug flow within two parallel planes with v parallel to the planes and the only relevant eigenvector normal to them.

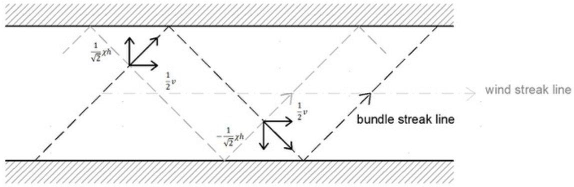

FIGURE 1. Plug flow due to bouncing.

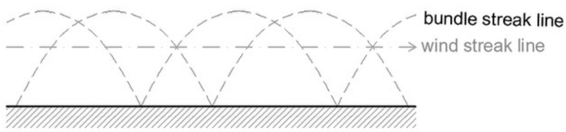

FIGURE 2. Bouncing on a horizontal plane of heavy molecules.

The second a similar flow but over a single horizontal plane of molecules as though they were acted upon by gravity. The third a sort of avalanche sliding, as though under gravity, over an inclined plane.

As already said we leave to the reader the task of filling necessary complements. We restrict our account to the train of thought leading to the motion as envisioned on Fig. 1. Suppose that L and B be both null, but H be not null. Then v and G have the same value everywhere, though the motes flow against each other in a mass balanced mode; the gross motion is one of bare translation (say, a “plug flow" in a channel). Imagine the flow in a plane containing v. Possibly the flow of a fluid occupying the slab between two planes parallel to each other and to v; and observe the motion on a plane normal to the slab and, as said, containing v. Let h be the normal to the confining planes and restrict attention to the case when h is eigenvector of H and the corresponding constant eigenvalue χ^2 is the only non null one. Then the motion can be imagined as due to the bouncing of motes between the planes; at each place, two tribes of motes cross, equally populous, one with velocity $\left(\frac{1}{2}v + \frac{\chi h}{\sqrt{2}}\right)$, the other with velocity $\left(\frac{1}{2}v - \frac{\chi h}{\sqrt{2}}\right)$. At the point of contact only one bundle streak line transits and the shock offered by the confining planes causes a discontinuity of the otherwise penetrating addendum.

In Fig. 2 the medium, assuming to be affected by gravity, is supported by a horizontal plane and lives in a vacuous environment devoid of molecules. A sort of near surface tension impedes the molecules to escape; such effect being mirrored thus: the only non-null eigenvalue decreases in the approach to the surface and becomes null there.

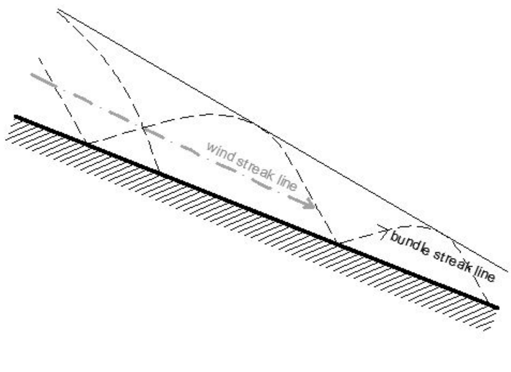

FIGURE 3. Avalanche of heavy molecules on an inclined plane.

Figure 3 feigns to represent an avalanche with the heavy medium flowing along an inclined plane but otherwise behaving as under the pretended conditions described above.

A final due remark stems from recalling that, within our speculations, molecules are supposed to be all alike; therefore undisturbed balanced cross-over, imagined above, may be replaced by internal bouncing at encounters and, consequently, streaks (smooth except for the recoils at the confining border) may be replaced by streaks zigzagging within each loculus, the bouncing velocity being given by $(\chi h/\sqrt{2})$. At the macro level the shocks cover the continuum.

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