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MODELS AND META-MODELS FOR INTERACTING PHENOMENA WITH SOCIAL FACTORS: A CONCEPTUAL PERSPECTIVE

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ABSTRACT. We often introduce regulatory constraints or behavioral indications to control or avoid diffusion processes with nontrivial social interactions. Examples are a pandemic or circumstances dealing with construction and management of civil structures, such as energy-dissipation reduction or the design, use, and installation of new classes of sustainable materials. The application of regulatory constraints by individuals fluctuates in rigor, depending on cognitive aspects and a number of additional psychological factors that influence decision making processes. These fluctuations may affect even drastically the previsions made through mathematical models of the phenomena under scrutiny. A basic question is as follows: How can we include such (say) psychological factors – or at least some estimates of them – into mathematical models for phenomena interacting directly with the social structure? A cascade of ancillary questions emerge. Among them: Do we need to consider such psychological factors just as a source of noisy accumulation to a bound – a stochastic approach, indeed – or in appropriate circumstances can we have a variational view on them interpreting context-driven effects as the result of the balance of opposite events? May we accept an approximate deterministic picture of these fluctuations, based, *e.g.*, on the introduction of continuous perturbations and/or memory effects? We indicate here a conceptual perspective to tackle such questions, and we formulate and discuss open problems.

From finitely many individuals to continuum schemes – reasons for connected pictures

Consider an assembly of several subsystems, each constituted by an ensemble of finitely many entities. To simplify a visualization of the circumstance, imagine that all these subsystems are replicas of a prototype, so that the analysis can be reduced to one subsystem and its interactions with neighbors. Essentially, we can have three circumstances:

1. The considered subsystem is isolated with respect to the ambient, and so are its replicas.
2. It is, instead, in energetic contact with the environment but remains closed to the exchange of mass.
3. It is fully open and its constituent entities may flow through its boundaries, while those of other systems can came in.

In the first case we say that we deal with a *microcanonical ensemble*. Second and third cases define what we call, respectively, *canonical* and *grand canonical* ensembles.

This classification is the starting point of classical statistical mechanics (see any book on this topic, from a classic one like Gibbs' treatise (Gibbs 1902), at least for the canonical ensemble, to more recent and updated volumes (Gallavotti 1999; Schwabl 2002)). It offers an approach to the analysis of the system sketched above that allows us to obtain information only in probabilistic terms, *i.e.*, looking at collective properties, rather than following the single individuals constituting the system itself. This view is general; it is irrespective of the nature of entities constituting the system under analysis. Per se can be considered as a meta-model.

When dynamics is dominant, approaches based on L. Boltzmann ideas appear to be appropriate. In short, Boltzmann's view goes like this: Imagine that the entities constituting the system are just molecules described by mass points interacting only through collisions and that their number is huge but finite – a gas, indeed. Boltzmann gave up following each individual molecule and chose a statistical approach. He took refuge in the velocity distribution function, which expresses the fraction of time that a given molecule, somewhere in space, has velocity in a given interval or the fraction of molecules that at a given instant have a certain velocity. In his 1872 fundamental article on this topic (*Weitere Studien über das Wärmegleichgewicht unter Gasmolekülen*, Wiener Berichte, 66, 275–370), Boltzmann made sure that both interpretations were possible. Then, he suggested that the variation in time of the distribution function is determined by collisions between molecules, and only by those collisions, and expressed formally such an idea in what we call nowadays the Boltzmann equation (see for details treatises such as the ones by Cercignani (1988) or Kremer (2010)). In choosing to describe in statistical terms the motion of the molecules of a gas, Boltzmann takes into account what characterizes gases, *i.e.*, the fact that each molecule in motion runs free space before colliding with other molecules, but essentially manages ignorance. He leaves out, in fact, the details of the dynamics of individual molecules, which he considers to be each deterministically governed by Newtonian mechanics, an aspect that could allow him at least in principle to follows each molecule, and manages to provide information about a system that otherwise would be difficult to analyze deterministically because of a procedural difficulty, unless we consider it as a continuous, that is made up of infinitely many innumerable molecules, although in this case we would disregard considering molecular free paths. Then, a question is to determine rigorously the continuous limit as the number of molecules goes to infinity. Arduous work is associated with it (see remarks in Saint-Raymond 2007). Of course, even in Boltzmann's picture, as in the description of ensembles above, that the colliding entities are molecules of a gas is a realistic and appropriate interpretation but it is just accidental: Boltzmann's scheme can be applied mode generally to systems constituted by finitely many individual entities, each free to move in space until it collides with other elements of the system, each described by the same variables, say placement in space and velocity through that placement at every instant in the time interval considered.

The pertinent continuum limit is a bottom-to-top procedure: we increment to infinity the number of molecules allowing them just to collide in principle in the same way along any direction, so, in the limit, we do not have internal energy due to molecular bonds, which are not accounted for. Further special assumptions may characterize the limit:

a. Molecules are small spheres with mass; smallness is left unspecified here but it is enormously tiny with respect to the region occupied by the full cluster of molecules. Also, they can collide in the same way and along any direction.

b. Each molecule may or not undergo homogeneous strain. In the latter case, at the continuum limit corresponding to full compaction of the molecules, if they fill completely a region and behave as a canonical system along the collective motion, we have a continuum that experiences only volume-preserving motion: it suffers the internal constraint of incompressibility.

c. Collisions may or not be dissipative.

Also, under the assumptions above, we may argue that the continuum limit should admit as a symmetry group the entire $SL(n)$, *i.e.*, the group of linear operators represented by $n \times n$ matrices (typically $n = 3$) with determinant equal to $+1$, a subgroup of the unimodular group modeled on the n-dimensional real space. Then, according to W. Noll's definition of material symmetries (Noll 1958), it should be a simple fluid, with no further option. So, without computing the limit of Boltzmann's equations, from previous physical considerations we may argue that, when collisions are conservative and molecules are rigid, the resulting continuum limit is a simple incompressible perfect fluid, appropriately described by the Euler equations. Furthermore, when the collisions involve friction, we get a viscous isotropic incompressible fluid so that the Navier-Stokes equations came into play. They also emerge from a stochastic view by considering the force (per unit volume) exerted by a molecule on the rest of a fluid over which it walks randomly. By averaging this force over an ensemble of such molecules and taking an appropriate limit, we may obtain the Navier-Stokes equations (the rigorous proof is in Peskin 1985). However, both the Euler and Navier-Stokes equations emerge when we leave a part the above mentioned bottom-to-top procedure and act directly at continuum scale, because that equations are deterministic in essence. Then, we get them simply as special offspring of the balance of forces, as it appears in the traditional format of continuum mechanics, under the reducing constitutive assumptions above listed. Also, once we have at continuum scale special forms of the balance of force and couples, specialized by the choice of appropriate constitutive structures, we can account for possible inherent stochasticity in the motion by considering random perturbations as fluctuations of bulk forces. However, even in the presence of a stochastic bulk perturbation, the resulting analysis may shift to a deterministic structure under appropriate circumstances. This is the case, for example, of the semi-linearized barotropic Navier-Stokes equations in a two-dimensional domain. When there are conditions under which we may consider the velocity as the gradient of a scalar function (a potential, indeed) and the stochastic forcing is itself the gradient of a special Wiener stochastic process satisfying the Ornstein-Uhlenbeck equation, the analysis becomes in essence deterministic (see Bessaih 2003 for the pertinent proof). This is not the only occasion of transition from stochastic to deterministic pictures; for example, some interpretations of quantum mechanics have this character (see, *e.g.*, Boström 2015). Although the stochastic view appears to be appropriate for the modeling of intricate phenomena in which we lack knowledge or an (at least apparent) intrinsic randomness seems to emerge, and stochastic methods may offer intriguing problems, for design purposes we need precise deterministic values the solutions of the equations characterizing a given model attain in certain circumstances.

Such values, however, can be reached with the ancillary support of probabilistic evaluations as it occurs in civil engineering design where the interplay between deterministic and probabilistic analyses is promoted in the EU rules to be adopted in the design of structures. Such an cooperation between deterministic and stochastic approaches is not limited to civil engineering design.

We find several examples of that fruitful interaction from quantum mechanics to condensed matter physics, even to mathematical psychology. However, let us come back to what we learn from the mechanics in classical space-time. If we look at spatial scales in a bottom-to-top view, *i.e.*, from atoms to tangible bodies of our daily experience, we realize non trivial cases of formation of structures at intermediate spatial scales that influence even drastically the gross behavior. Examples come from condensed matter physics: the entanglement of molecules in polymer suspensions, layers in smectic liquid crystals, stacks of disk-like mesogenic molecules containing no chiral center that characterize liquid crystals in cholesteric phase, shear bands in generic elastic-plastic bodies, clustering of microcracks up to macroscopic crack in brittle materials, etc.

Beyond the single human scales, we find clear circumstances of this type at the scale of the society. Think of example to a pandemic like COVID19. Its diffusion depends on whether the infected droplets emitted by an individual come into contact with the respiratory system of another organism; and we may describe the pertinent dynamics as the one of a fluid spread out in an environment with decaying velocity. A family, a class in a school, a village, a city are structures at a scale smaller than the one of a region, a state, a bigger society including multiple national entities linked by some type of agreement — so we can call a family, a class in a school etc. as substructures or microstructures, depending on convenience and the scale we look at. The behavior of one or more substructures may influence drastically the pandemic diffusion and its (say) intensity, or it may be a fluctuation reabsorbed after applying appropriate confinement conditions.

A question emerges: At continuum scale (and just thinking in deterministic way) how can we describe such multiple scale interactions in terms of meta-models, *i.e.*, without looking at a specific class of phenomena, rather thinking of a model-building framework?

Once again, continuum mechanics in classical space-time suggests an answer; however, more than its traditional format we need to look at its multi-field refinement: the general model-building framework of the mechanics of complex materials.

Multi-scale views imply multi-field representation of phenomena

Continuum mechanics rests on a conceptual hierarchy in which every step is independent of and influences the subsequent one. Such a hierarchy goes as follows:

i. Representation of the body morphology and its changes.

ii. Characterization of observers and their changes.

iii. Representation of interactions and derivation of the pertinent balance equations.

iv. Choice of the state functions, the so-called constitutive structures.

The first item above, the step that opens a modeling process, seems to be at a first glance just a matter of an introductory chapter of differential geometry. Indeed it is apparently just so from a formal viewpoint. In fact, opening their 602 page long article on the *"Handbuch*

der Physik" Truesdell and Noll wrote that "a body is a three-dimensional differentiable manifold, the elements of which are called particles" (Truesdell and Noll 2004, p. 37). With this, they were in agreement with A. S. Lodge, quoted in a footnote, who wrote "it is clear that we have to deal with one continuous geometric manifold (the medium) immersed in and moving through another one (space); we shall refer to these as the 'body manifold' and the 'space manifold', and we shall call points of the two manifolds 'particles' and 'places' respectively" (Lodge 1964).

This starting step, however, presumes a decision on what we think a body is. "A continuous body is a set B of points called material points" wrote M. Šilhavý in his 1997 treatise (Šilhavý 1997, p. 29). Accordingly, we could say that a body is a set of so-called material elements, which are left unspecified unless vaguely thinking that they are "the smallest portions of a material to exhibit certain of its distinguished properties" (Truesdell and Toupin 1960, p. 226). Then, the key question is to give geometric structure to this abstract set, a structure linked with the physical evidence of the body or the class of bodies under analysis. The traditional choice of considering such a set to be represented by a three-dimensional differentiable manifold, embedded onto a fit region of the three-dimensional real space, namely a bounded, open, connected region, with surface-like boundary oriented by the outward unit normal to within a finite number of corners and edges, is minimalistic and also necessary for analytical reasons. The geometrical choice that we do is, in fact, a representation of the material morphology. Selecting only a fit region implies that we are considering the material elements as indistinct pieces of matter, a sort of black boxes, and we give information on their structure only at a later stage, when we consider material symmetries. At the geometric level of representation of the body morphology, we just select a domain in space where we define continuous fields at macroscopic scale, looking directly only at it. They are deformations and related interactions, defined by the power that they perform on the rate of change of a the material morphology. Managing such fields we assume implicitly that what they describe is indefinitely divisible without losing any of its defining properties. In this way we disregard intermediate structures given by physically occurring molecular bonds into clusters at mesoscopic or microscopic spatial scales with peculiar properties due to the cooperation among the constituting material elements. We have already quoted a few peculiar examples. We could add several other examples, one for all is the case of fluids with clustering pollutants, which has non-trivial interest for environmental analysis and related social impact.

A way to account for intermediate structures at small spatial scales is to consider material elements as systems, rather than black boxes, introducing a description of such systems.

The germ of this idea apparently emerged from W. Voigt's suggestions to Eugène and François Cosserat. The two brothers formulated in 1909 a theory of elasticity in which every material element was considered as a tiny (smallness left unspecified) rigid body able to freely rotate with respect to its neighbors. That proposal remained not further explored until in 1958 J. L. Ericksen and C. A. Truesdell adopted it for dimension-reduction models of elastic structural elements, namely beams, plates, shells (Ericksen and Truesdell 1957). Earlier, the use of descriptors of mesoscopic structures (say, order parameters or phase fields) were introduced since 1937 by L. D. Landau to represent second-order phase transitions (*i.e.*, those involving material symmetries such as it occurs in martensitic-to-austenitic or paraelectric-to-ferroelectric phase transitions).

Such an approach progressively became a paradigm in solid-state physics to describe ordered media (Mermin 1979), but it was followed without considering in general the coupling with the macroscopic strain or at least taking into account small strains only (as in the case of ferroelectric materials (Salje 1991)). Exceptions emerged in the theory of liquid crystals as proposed in the early 1960s by J. L. Ericksen and developed also by P. G. De Gennes (de Gennes and Prost 1995). Then, in 1964 R. D. Mindlin extended Cosserat's view by considering every material element as something able to undergo micro-strain independently of its neighbors, an approach largely developed since then by various authors (see, among related works, Eringen 1999; Neff 2006). A multifield scheme was also used for porous (Nunziato and Cowin 1979) and polymeric bodies (Doi and Edwards 1978), and for damage evolution (Frémond and Nedjar 1996; Mariano and Augusti 1998; Bisconti *et al.* 2019).

However, besides specific cases, the list of which we could enlarge further, a basic question was whether we can have a unified view on that approaches describing interacting phenomena at various scales in materials (those we call complex to recall in short the presence of – say – active microstructures influencing the gross behavior). Can we construct for complex materials a meta-model working as a model-building framework? A path towards a positive answer to such a question was opened in the late 1970s by G. Capriz. The basic idea of his unification program is to couple deformation maps and descriptors of the low-spatial-scale material morphology viewed generically as elements of a finite-dimensional abstract manifold $\mathscr{M}$ (Capriz 1989), what we can call here a manifold of microstructural shapes. Capriz developed the approach, among others, with P. Podio-Guidugli (Lagrangian structures and internal constraints), E. G. Virga (algebra of bodies and representation of interactions), P. Giovine (inertia and sparse media), P. M. Mariano (Hamiltonian structures, junctions, and sparse media). Then, the last author developed procedures for the derivation of pertinent balance equations from invariance principles, showing how in general microstructures influence the evolution of defects (Mariano 2002, 2014). In the static elastic case under a large strain regime, existence of weak solutions in the unified framework has been proven in 2009 (Mariano and Modica 2009), a result refined to include multiple-valued descriptors (Focardi *et al.* 2015), or vector-measure-valued descriptors of the material morphology as representative of crack paths (Giaquinta *et al.* 2010). The resulting theory includes as special cases Cahn-Hilliard and Ginzburg-Landau ones, but also all the current phase-field models (Mariano 2002; Miehe *et al.* 2016).

Consequently, if we can back to what discussed at the beginning of this section, we are shifting from a representation of bodies as three-dimensional manifolds embedded into the three-dimensional real space to a view considering a body as a fiber bundle having as a basis a fit region in the three-dimensional real space, a region moving in that space, as in the traditional view, and typical fiber the manifold of microstructural shapes. Configurations are composed by sections of such a bundle, speaking in the terms of differential geometry. Does such an appropriate multi-field picture for complex materials be extended to cover in general, so beyond materials at continuum scale, interacting phenomena with social factors?

A possible path to follow

Consider a system of several (finitely many) individual entities distributed in a region of space and able to move within it. Consider a smaller region, a window in space, a box of side δ, the scale at which we accept to make averages attributing the results to values of continuous fields. We write $\mathfrak{e}(x)$ for a window the statistical properties of which we attribute to the point x at instant t. The cluster in $\mathfrak{e}(x)$ should be so populous to assure the possibility of statistical estimates beyond averages.

Let us assume to know a distribution function $\Theta(x,t;y,w)$ giving the number of individual entities that are at the instant t in an infinitesimal neighborhood of a point in $\mathfrak{e}(x)$ individuated by the vector y issued from x and are endowed with a property w, which we presume to be read on a linear space V. The choice of considering w to be an element of a generic linear space is essential, otherwise the definition of some averages could be meaningless.

The simplest choice for w is to be the velocity of particles of the same type, all endowed with the same mass, a choice adopted in a multi-scale view on granular clusters (see Capriz 2008; Capriz and Mariano 2014; Capriz and Giovine 2018; Capriz and Mariano 2018, 2019), which we extend here to cover general systems with interactions across spatial and temporal scales. With this aim, we can consider w to be a pair composed by the velocity of a given individual and a property (or a list of properties) pertaining to it, provided that w be read always in a linear space. The average v of w over the entire window and the local average of w at y can be computed. We thus have

$$v(\tau,x) := \delta^{-3}\int_{\mathbf{e}(x)}\Big(\int_V \Theta(t,x;y,w)\,w\,\mathrm{d}w\Big)\,\mathrm{d}y\,,$$

and

$$w_*(t,x;y) := \left(\int_V \Theta(t,x;y,w)\,\mathrm{d}w\right)^{-1}\int_V w\,\Theta(t,x;y,w)\,\mathrm{d}w,$$

Then, we take for the local average of w the additive decomposition

$$w_* = v + By + c\,, \tag{1}$$

where B is a linear operator defined by

$$B = \arg\min_{x\in\mathscr{B}}\int_{\mathbf{e}}\Big(\int_V \Theta(t,x;y,w)\,\mathrm{d}w\Big)(|w_*|^2 - |v+By|^2)\mathrm{d}y,$$

for every x and t. The linear operator B describes an affine component of the fluctuations with respect to v, while c represents spurious fluctuations. We imagine to describe the (abstract) system under analysis by using as basic fields v and B considered independent at first glance, coupled by the balance equations of interactions associated with them. They must contain time derivatives of v and B that are objective in the sense that they are Lie derivatives dragged by the relative evolution between v and B (in the case in which w represents a velocity see Capriz and Mariano 2014 for details and rigorous definitions). A linear operator, say G, is associated with B. It is solution of the differential equation

$$\dot{G} = BG$$

where the superposed dot means time derivative.

When v is differentiable in space, another linear operator, say F, may be associated with its gradient, as solution to the differential equation

$$\dot{F} = (\nabla u)F \ .$$

A simplified case is when there is some reason to impose the internal constraint $F = G$. When w represents just the velocity of a mass point, such a constraint implies that, from a statistical viewpoint, we are considering the window as a canonical system, not open to the exchange of individual entities with the environment. In this special case, the balance equations - obtained by requiring the invariance of a linear functional of v and B, namely the external power exerted over a generic compact portion of the region occupied by the system - reduce to the equations

$$\begin{aligned} v_t + (v\cdot\nabla)v + \nabla\pi + \mathrm{div}\big(H - \big(\nabla v_t + (v\cdot\nabla)\nabla v\big)Y\big)\big) = \\ \mathrm{div}\big(\bar{\mathbb{C}}\nabla u - 2(\mathrm{div}(r_1\nabla\mathrm{sym}\nabla u + r_2\nabla\mathrm{sym}\nabla v)\big)^{\top}\big) + f, \end{aligned} \tag{2}$$

$$\mathrm{div}v = 0, \tag{3}$$

$$H_t + (v\cdot\nabla)H = J, \tag{4}$$

$$Y_t + (v\cdot\nabla)Y = \nabla vY + Y\nabla v^{\top}, \tag{5}$$

where

$$Y(x,t) := \delta^{-3}\int_{\mathfrak{e}(x)}\Big(\int_{\mathbb{V}}\Theta(t,x;y,w)\,\mathrm{d}w\Big)\,y\otimes y\,\mathrm{d}y\ ,$$

and

$$H(x,t) := \left(\int_{\mathfrak{e}(x)}\Big(\int_{\mathbb{R}^3}\Theta(t,x;y,w)\,\mathrm{d}w\Big)\,\mathrm{d}y\right)^{-1}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\Theta(t,x;y,w)\,\mathrm{d}w\,c\otimes c\,\mathrm{d}w\,.$$

The linear operator H is a collective indicator of the spurious (in the sense of hardly controllable) fluctuations. J is the source of such fluctuations, as f is an external action performing power over the average velocity v.

Some open problems

Even in this simplified case, an analysis of the system above is a challenging task. Problems emerge.

- Under which conditions do solutions to the previous system exist under appropriate initial and boundary conditions? For them, do we need to introduce some regularizing terms, passing eventually to the limit as these terms disappear?
- If we find existence, what can we say about the possible decaying behavior of the solutions?
- Assume that the source of spurious fluctuations are due to social factors, how can we model them? Specifically, according to suggestions coming from neuroscience, do we need to model J as a stochastic process of Wiener type (Srivastava *et al.* 2017) or, else, could it be appropriate to consider it as a solution of an independent stochastic functional equation (Turab *et al.* 2022)?
- What would we lose or gain if we considered J as emerging from a potential, according to proposals like the one in reference (Gronchi and Provenzi 2017)?

Of course, the same questions and ancillary ones emerge when we avoid restricting ourselves to the simplified case $F = G$ and consider the full version of balance equations. We can embed in them memory type effects, above all those with kernel given by a gamma-function, which allows one to describe circumstances in which a critical event in the past influences the present dynamics more than previous and intermediate events. Existence and regularity problems emerge from the analytical viewpoint. In addition, nontrivial modeling issues emerge as, above all, in the case of memory, the link between the structure summarized above and the crop of memory models coming from neurosciences and psychology of learning, at least looking at tentative of unification in that sector, as the one proposed in reference (Kelly *et al.* 2017).

The scheme can be further extended considering the system homogenized in the way summarized above as embedded into another continuum system. This is the case, for example, of pollutants suspended in a ground fluid, a case discussed by Mariano (2020). In any case, to the best of our knowledge, we do not know similar approaches available in literature to interacting phenomena with social factors.

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