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Why a mechanistic theory of soils is crucially important: Another line of supportive arguments exists, seldom invoked in soil science

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Abstract. In the last few decades, the sizable effort that has been devoted to the mechanistic, quantitative description of soil processes has been justified on the grounds that theories and models help us understand how soils function, and also predict how, e.g., they are likely to adjust in the future to environmental change. The argument, familiar to physicists, that theories uniquely determine what should be measured has rarely if ever been invoked in the soil science literature. On the contrary, to enable the classification and mapping of soil, enormous amounts of "theory-free" data have been and continue to be amassed by soil scientists. In this general context, the key objective of the present Forum article is to argue that the accumulation of more "theory-free" data, in particular to allow the application of artificial intelligence methods, is not sensible at this stage, and that the development of improved theories of soil processes is crucial, to provide guidance about the type of measurements that should be performed. Hopefully, this Forum article will stimulate a debate on this issue, and will lead to a much needed intensification of theoretical research and modelling in soil science.

1 Introduction

Over the last few decades, a very significant research effort has been devoted to the development of mechanistic theories describing some of the physical, (bio)chemical, and biological processes taking place in soils (see review, e.g., in Vereecken et al., 2016). These theories have led to the emergence of an impressive array of computer codes, using a variety of numerical approaches. Several authors, in recent years, have called for an intensification of the research in this area, toward the development of a "theory of soils" (e.g., Neal, 2021; Neal et al., 2021)

In their justification of the need for theory and model development, researchers in soil science have traditionally relied on one of two lines of arguments. The first is that by trying to encapsulate into a mechanistic theory what we know about a given process and by comparing computer model outputs with experimental data, it is possible to assess whether our knowledge appears to be satisfactory or is missing some important component of reality. From this perspective, theory building assists the discovery process. Another argument is that theories, and especially the computer models they lead to, help us predict how soil processes are likely to evolve in the future, in the context of climate change (e.g., Chalhoub et al., 2025) or as we try to determine which soil management practices are beneficial to address mounting demands on soils (e.g., Ray et al., 1996).

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An additional line of arguments, commonly adopted in other disciplines, appears to have rarely made any noticeable foray into the soil science literature. It considers that mechanistic theories are absolutely necessary to determine what needs to be measured. This perspective is frequently embraced in physics, among other fields of knowledge. Decades ago, Einstein (quoted in Salam, 1990) opined that theory "decides what can be observed", and by extension, what cannot. For instance, Heisenberg's indeterminacy principle states that one cannot measure both the position and momentum of a particle, such as a photon or electron, with perfect accuracy; one has to choose one or the other. In addition to spelling out clearly what can and cannot be measured, a theory also points out the parameters it makes sense to measure, and, by default, those that are irrelevant. For example, because the theory we rely on to accurately describe the thermal expansion of metals under usual environmental conditions involves ambient temperature but not the CO_2 concentration of the air, we know that measurements of the former are crucial to predict in practice by how much above-ground electrical cables are likely to elongate in the Summer, whereas measurements of the latter are not useful at all.

In this general context, the primary objective of this Forum article is to stimulate a debate on the perspective that mechanistic theories are crucially important in soil science as well, to determine what characteristics of soils we need to measure in order to manage soils properly and to design appropriate experiments to test specific hypotheses. To put the narrative in a proper framing, I first try to understand why, in soil science, this line of arguments in support of theory development appears to have rarely if ever been alluded to.

2 Historical reliance on "theory-free" data in much of soil science

When in mid-19th century, scientists started paying serious attention to soils, they were immediately confronted with their enormous spatial heterogeneity, requiring ways to classify and map them. To that end, given the sizeable task at hand, measurement methods were needed that at the same time were rapid, could be implemented directly in soil pits or in a rudimentary field laboratory without requiring sophisticated equipment, and dealt with static properties of soils, which did not change appreciably over time. The granulometry of soils, the depth, color, and apparent organic matter content of horizons, or the average size of "aggregates" were among these easily measured parameters and have constituted the basis on which soils have been mapped for over a century and a half. Their measurements do not require any underlying mechanistic theory of soil processes, either to design the data-acquisition methodology or to interpret what the data imply. For a long time, there was very little theory of soil processes to speak of anyway, which could have been used to design measurement methods, except in relation to the movement and retention of water in soils, but the associated measurements were far too laborious and time-consuming to be used for soil mapping over large regions.

When, after the 1960s, soil survey campaigns got completed in a number of countries, and interest among soil scientists tended to shift to the multitude of soil processes responsible for the multifunctionality of soils (Simonson, 1966; Heuting, 1970), it became rapidly evident that "theory-free" soil data gathered for the purpose of soil classification and mapping would no longer be adequate. A vivid example of that involves the cation exchange capacity (CEC) of soils, which, for purposes of soil classification, had traditionally be measured via replacement of exchangeable cations with a saturating solution at a set pH of 7 or 8.2 (e.g., Sumner and Miller, 1996). This standard measurement technique produces results that do not make much sense when one attempts to describe soil processes, because under undisturbed conditions in soils, the pH often differs from those set values, and because, as shown experimentally by a number of researchers (see, e.g., Mokady and Bresler, 1968; Boast, 1973; Barton and Karathanasis, 1997), the actual CEC of a partly water-saturated soil differs from that obtained when the soil is fully water-saturated.

Nevertheless, the idea emerged in part of the soil science community that the mass of "theory-free" data that by then had been accumulated could be useful to describe soil processes, provided one could establish reliable statistical correlations between these data and the various "difficult to measure" dynamical parameters needed in that context. This idea led some researchers to develop so-called "pedotransfer functions" (see, e.g., Bouma, 1989; Bouma et al., 1996, 2022; Weijnants et al., 2009; Vereecken et al., 2010). One could argue that the work on pedotransfer functions has legitimated the continued acquisition of "theory-free" data, and the recent strong push to digitize soil maps globally, to make them more accessible to users. The idea that theory-free data suffice for most practical purposes has also led some soil researchers to advocate that research on soils could be "data-driven", e.g., using data-mining, machine-learning, or Artificial Intelligence (AI) techniques (Bui et al., 2009; Bui, 2016; Chen et al., 2019; Wadoux et al., 2021; Wadoux, 2025; Minasny and McBratney, 2025; Teodosio et al., 2025). The hope in this context was that these approaches, for whose "training" massive amounts of data are needed, could present a significant potential to address and answer successfully some of the key questions about soils with which we are confronted

It is not clear at this stage whether these approaches still hold the same "potential for advancing knowledge and innovation" (Wadoux, 2025) they were claimed to have not very long ago. Indeed, they have clearly run into a serious snag. Starting with Fourcade et al.: 2018), various authors have demonstrated that statistically stronger patterns can emerge from databases to which one has deliberately added entirely irrelevant information, for example, a painting or the photograph of a colleague (Behrens and Viscarra Rossel, 2020; Wadoux et al., 2020; Rentschler and Scholten, 2025). Clearly, machine-learning and AI techniques are not able at all to discriminate on their own between what is meaningful information and what is not. This is hardly surprising since these methods rely heavily on correlations, which we know are intrinsically not informative at all about causation. Rentschler and Scholten (2025) conclude from it that users have the responsibility to make sure that parameters they consider when implementing these techniques are "in line with existing scientific theory of mechanistic and process understanding". In other words, after decades of trying with a variety of statistical and, lately, AI approaches to rely on masses of "theory-free" data to describe soil processes and functions instead of spending time developing dedicated theories or computer models, it appears necessary to backpedal, and to address head-on the fundamental question of what data we actually need, i.e., which ones are directly relevant to what we want to do.

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3 A theory is needed to determine which measurements are relevant

Perhaps the most persuasive plea for the crucial importance of theory in that context comes from the literary world. In her 1923 novel "Murder on the links", which I think should be recommended reading for all soil science students, Agatha Christie contrasts the modi operandi of two detectives. A French detective runs around feverishly, painstakingly amassing all kinds of information, whereas the famous Belgian detective Hercule Poirot (who, of course, ends up solving the case) mostly sits in an armchair, trying to elaborate a theory of the murder. Poirot's philosophy is that, past a certain point in a murder investigation, one does not know whether a given bit of information is a clue or, even more basically, where to look to gather additional information in a time-efficient way, unless one has a guiding theory.

The early history of soil physics provides a vivid example of the soundness of this perspective. Buckingham (1907), starting from first principles in physics, developed a theory of water movement in unsaturated soils that led him for the first time to identify the soil water matric potential, the soil water retention curve, and the unsaturated hydraulic conductivity as essential properties of soils in that context (e.g., Nimmo and Landa, 2005; Narasimhan, 2007). At the time, equipment was entirely lacking for their measurement in the field. The first tensiometer, enabling the measurement of the soil water matric potential, was developed a year later, in 1908 (e.g., Or, 2001). Had it not been for Buckingham's (1907) theoretical work, soil physicists might have continued for a long time to try to cope with the description of water movement using easy-to-measure, "theory-free" properties, like soil texture or aggregate size, which his research showed clearly to be irrelevant to the description of soil water movement.

This example could serve as a blueprint for how to proceed in other areas of soil science. For instance, there is a lot of interest at the moment in the effect that bacteriophages could have on various soil processes, like the mineralization of soil organic matter (SOM) and the resulting emission of greenhouse gases by soils (e.g., Pratama and Van Elsas, 2018). Estimates are that there are 10 times as many bacteriophages as bacterial cells in soils, so their so far largely unknown overall effect could be significant. Should we account for it explicitly when we try to predict the fate of SOM? To answer this question, the traditional approach in soil science would have us measure everything we can about bacteriophage abundance and diversity in soils, after which we would try to determine statistically if these data are correlated significantly to processes of interest. This would require an enormous amount of work, likely spanning many years and forcing us to measure a large number of parameters that might turn out eventually not to matter. By contrast, a theoretical approach would consist of developing a model of bacteriophage action in soils, based, e.g., on what is known about the behavior of viruses in other systems, and about the dispersion in soils of nanoparticles similar in size to phages. The hypotheses embodied in this model could be tested in simple targeted experiments involving one or two bacteria-bacteriophage pairs, either in actual, sterilized soil samples, or in 2D micromodels. This model, once tested, could then be incorporated with the description of other aspects of soils (see Figure 1) to obtain a comprehensive theory. In many ways, the same approach should be adopted with respect to taking soil fauna explicitly into account (Briones, 2014, 2018; Cayuela et al., 2020).

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Realistically, the development of this comprehensive theory is not going to be straightforward. Many questions still remain unanswered at the moment about the proper framework for this work. Ecosystem-scale models have assumed for a long time that SOM could be apportioned into separate pools with distinct turnover times, and that its mineralization kinetics could be described by simple first-order reactions, without explicitly accounting for the presence or activity of microorganisms. Efforts have been made in the last two decades to introduce features in the models that deal explicitly with microbial action, carbon use efficiency, and priming, but proponents of this approach admit that they are still largely struggling with it (e.g., Schimel, 2023). A very different, "bottom-up" approach, stimulated by the commercialization of table-top X-ray scanners twenty years ago as well as progress with a number of spectroscopic and pore-scale modelling techniques, consists, as in Figure 1, of developing a model of soil carbon dynamics on the basis of observations of soil processes at the microscale, commensurate with the scale at which microorganisms operate (e.g., Baveye et al., 2018; Pot et al., 2021, 2022a,b). A serious challenge in this context is the need to upscale the description of processes from the micro- to the macroscale, although this still largely unresolved upscaling hurdle occurs no matter which approach, top-down or bottom-up, is adopted (Baveye, 2023). Another challenge is that some of the parameters that the microscale modelling indicates should be measured, like the average spatial separation between microorganisms and SOM (e.g., Mbé et al., 2022), cannot be measured directly at the moment, so that alternative routes to these parameters need to be found. To resolve some of the pending issues, we need a concerted research effort over the next few years. This effort, by definition, needs to be interdisciplinary and therefore requires a break with the very much mono-disciplinary focus that continues to dominate soil science (e.g., Baveye and Wander, 2019; Baveye et al., 2024).

4 Take-home message

In this forum piece, I have argued that soil scientists should discontinue the long-standing practice of accumulating masses of "theory-free" data and of attempting to correlate them to processes of interest. Numerous examples in physics, including in soil physics with the work of Buckingham (1907), show that we need theories to determine which parameters have to be measured in order to describe dynamical soil processes quantitatively, and ultimately manage them properly. We have some theories already for specific situations, and significant progress has been achieved in recent years toward the development of a comprehensive theory of physical, (bio)chemical, and microbiological processes in soils, but a lot more work remains to be done in the area, in particular to better take into account a number of aspects that have been neglected in that context so far, like plant-soil relationships, and the effect of soil fauna or bacteriophages. The hope at this stage is that the sustained debate this article is trying to stimulate on the need to develop new theories will help determine which theoretical framework is most suitable for this work, and will convince soil scientists that a significant interdisciplinary effort is in order rapidly.

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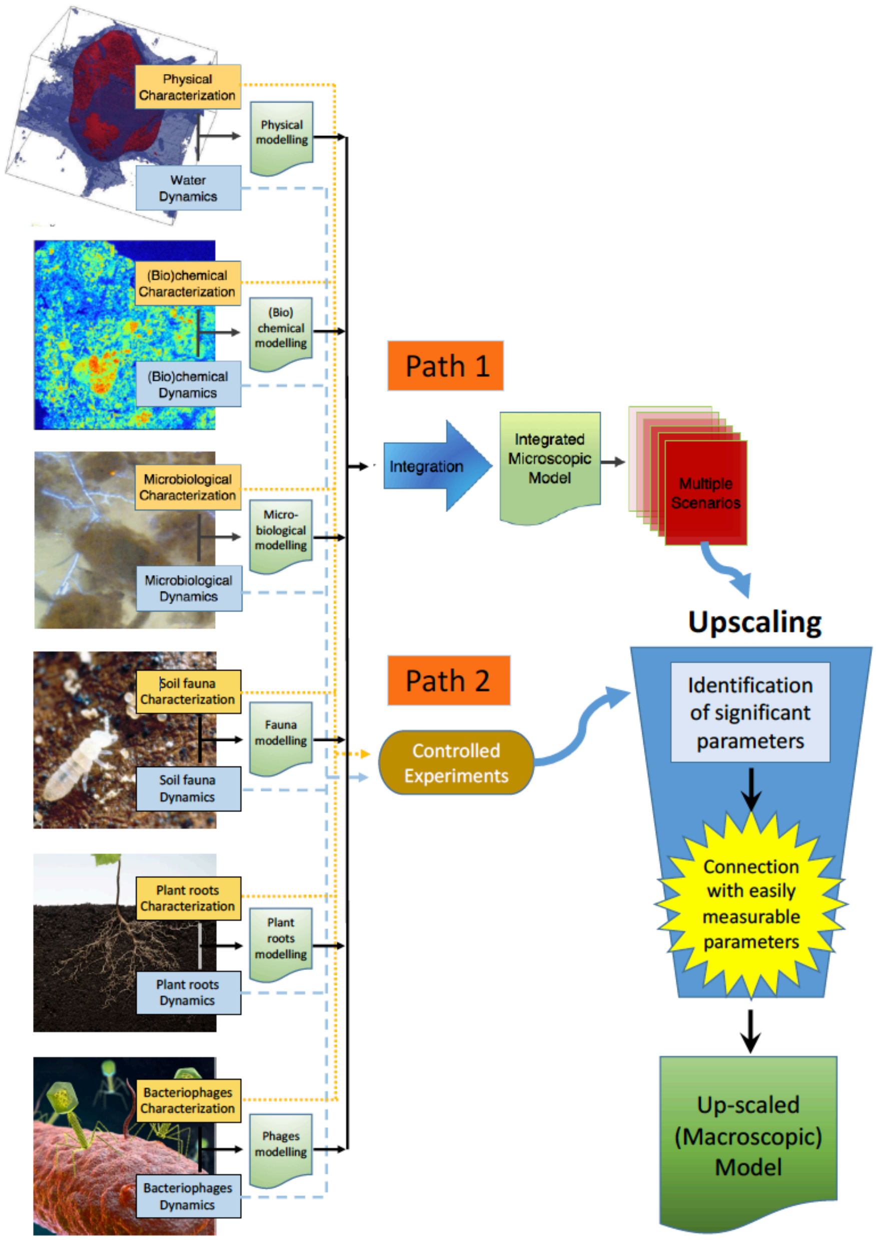

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Figure 1: Schematic representation of a possible sequence of steps in the development of a model of soil carbon dynamics applicable to large (macroscopic) spatial scales, starting on the left from a characterization of the static (light brown boxes) and dynamic (light blue boxes) components of different properties of soils at the microscale. The green boxes correspond to initial (left), intermediate (center), and final (right) modelling efforts. Following path 1, the integration of different perspectives results in the development of a microscale model of soils, which can be run multiple times, under a variety of scenarios. Along path 2, controlled experiments are carried out to obtain macroscopic data against which microscale measurements on soil samples can be contrasted. These data, in parallel with the outcomes of scenario modelling, feed into the upscaling step, whose goal is to identify easily measurable macroscopic parameters associated with an up-scaled model (Baveye, 2023).

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