MULTISCALE PLASTICITY: REDUCTIONISM OR EMERGENCE?

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Summary During the twentieth century, a multiscale picture of plasticity has emerged that links macroscopic plasticity, expressed in yield functions and flow rules, to the carriers of plastic deformation: dislocations. The multiscale paradigm comes in two flavours: a rather idealized and seldomly practiced approach where the behaviour of smaller scales is embedded in that of the next size scale, and the more common one where understanding from smaller scales is used to inform higer-scale models. In either form, multiscale plasticity is sometimes viewed as the 'complete theory of plasticity'.

But, is it? And, if not, is this just a matter of time and continued research efforts? In this talk I will attempt to address such questions by confronting a reductionists point of view with one based on the notion of emergence.

INTRODUCTION

The twentieth century has witnessed the growth of various new branches on the tree of Solid Mechanics. Plasticity is one of them.

Plastic deformation has been studied at different length scales, as illustrated in Fig. 1, but not in any particular order. It is interesting to note that the extreme ends of the size scale picture emerged at about the same time. Macroscopic yield criteria were first formulated by Huber and Von Mises in the early 1900's, around the same time that Volterra gave his first mathematical description of dislocations , objects that were only first suggested by experiments just before the turn of the nineteenth century. The size scale gap between these scales was gradually filled by the development of crystal plasticity, based on early work by Taylor in the 1930's but only becoming a practical tool in the 1980's with the advent of powerful computing.

At present, where a convincing body of knowledge has been attained at each of the scales in Fig. 1, it might be tempting to conclude that we have a 'complete multiscale theory of plasticity'. But, is it? – complete and multiscale? This paper will address these questions by confronting the theory with (somewhat philosophical) notions of reductionism and emergence.

MULTISCALE PLASTICITY

The popular multiscale modeling paradigm comes in two flavours: a rather idealized and seldomly practiced approach where the behaviour of smaller scales is embedded in that of the next size scale, and the more common one where understanding from smaller scales is used to inform higer-scale models. In the context of Fig. 1, the first approach could be paraphrased as 'from large to small', and the second by the opposite – 'from small to large'. These two approaches are not equivalent but are pointing towards the more formal, and more insightful, concepts of reductionism and emergence.

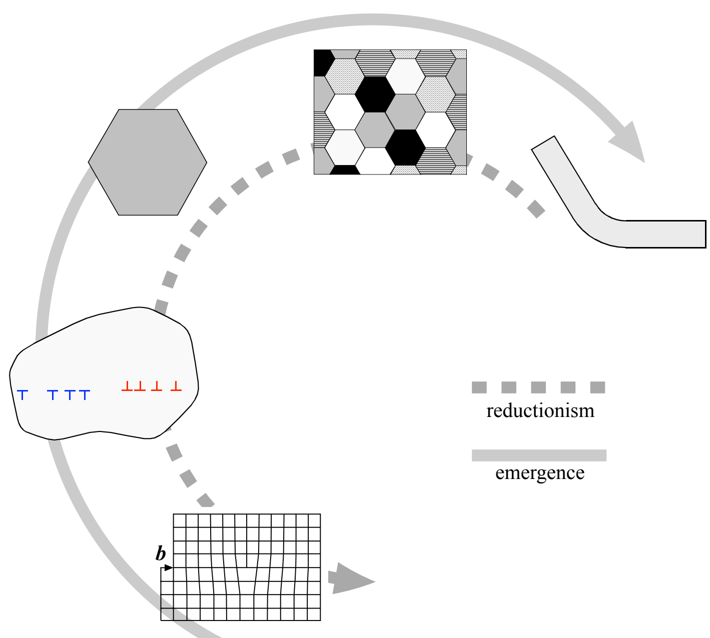

Figure 1. *Schematic of plasticity at various length scales.*

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A reductionist view of plasticity

Many people hold the view that science and engineering is about disecting a complex problem into smaller components that can be analyzed. If that component is still complex, you break it up into even smaller pieces, and so on. A true reductionist would keep going down, hoping that, eventually, he will find a component that is simple enough for him to understand. Thus, the reductionist point of view on plasticity is that, in the end, it boils down to the behaviour of dislocations in the atomic lattice of a material.

But what is meant with "understanding" in the above? That we can explain what it is that causes plastic deformation? Or that we can predict how the plastic deformation of a macroscopic component depends on the atomic arrangement? If we recall that there are on the order of 10^{19} to 10^{20} atoms in a cubic millimeter, nobody will expect that we can explain the plastic deformation of even a simple object as a paperclip by knowing the positions of all atoms.

This can be avoided if we call "understanding" when the macroscopic behaviour is explained in terms of an intermediate-level description. But how do we arrive at that level?

Emergence

In his inspiring book *The Fabric of Reality*, Deutsch defines 'emergence' as "high-level simplicity 'appearing' from low-level complexity" [1]. This does sound a lot like multiscale plasticity! At each of the size scales in Fig. 1 from atomistics (lower left-hand corner) to the macroscopic scale of a specimen (top right-hand corner) there is emergent behaviour: dislocations as the collective mis-placement of atoms in a lattice; crystallographic slip inside single crystals due to the collective motion of dislocations; texture development by cooperative lattice rotation; deformation-induced anisotropy at the macro level.

Each of the above steps in emergence has two correlated characteristics: reduction of the number of degrees of freedom and the introduction of new coarse-grained degrees of freedom with associated constitutive equations. It is important to note that the higher the level of observation in the plasticity hierarchy, the more abstract the degrees of freedom become, both physically and mathematically. While the behaviour of dislocations at the atomistic level can be described basically by $F = ma$ applied to points, macroscopic continuum models are phrased in terms of complex relationships between the strain-rate and the stress tensor, involving fourth-order orientation tensors.

THE ULTIMATE THEORY OF PLASTICITY

In this talk I will argue that the current theory of plasticity is neither a purely reductionist's view nor based on emergence. In fact, rather than 'multiscale plasticity' it even seems more fair to speak of 'plasticity at multiple scales'. The multiple scales shown in Fig. 1 give some structure to the different faces of plasticity in the sense of ordering, but it is not a structure in the sense of layers built on top of other layers of knowledge. In principle, a polycrystal theory of plasticity could be 'derived' from a single crystal theory, and a single crystal continuum theory could be 'constructed' on the basis of discrete dislocation plasticity, etc. .... but, apart from certain aspects, these formal scale transitions have not been performed.

In an ideal world, an emergence-based theory of plasticity would be a true multiscale description starting from the atomic level, with subsequent higher-length scale models emerging by appropriate coarse-graining. Such an approach has been explored in the last decade for the scale transition of discrete dislocation plasticity to continuum crystal plasticity. It has taught the mechanics community that there is more to scale transitions than 'volume averaging' (as the ruling paradigm in micromechanics). The key is not only to eliminate the irrelevant degrees of freedom, but also, as is well known in statistical mechanics, to transfer this 'loss of information' to the next scale in some form of entropy. How this entropy should propagate up the size scale ladder is a major challenge.

References

[1] D. Deutsch, *The Fabric of Reality*, Allen Lane, The Penguin Press, 1997.