Comparison of computational methodologies for predicting plastic activity in amorphous materials

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Imposing an external driving, amorphous solids can flow via a succession of plastic rearrangement of localized particles. Numerous numerical and experimental studies have shown that loci of plastic instability in glasses are triggered by spatially localized soft spots in direct analogy with dislocations present in crystalline solids, although the population and microscopic structure of the former being significantly different from the latter. The detection and nature of such “amorphous defects” have received a lot of attention, one of the goals being to predict from the microscopic structure itself which regions are likely to undergo a rearrangement upon deformation.

I will present various structural indicators ranging from purely structural to highly non-linear methods that require the knowledge of the interactions between constituents. I will discuss in detail indicators that are constructed from an analysis of the potential energy landscape and present novel anisotropic descriptors that take into account the tensorial nature of the coupling between soft spots and loading geometry.

***Bio**: David Richard did his PhD in Mainz (Germany), where he worked on rare event sampling methods to model nucleation phenomena. He is now working within the Simons collaboration on "cracking the glass problem". His research is focused on understanding the statistics and micromechanics of quasi-localized excitations and their role in controlling the dynamics of supercooled liquids and the failure of driven amorphous materials.*