From particles to continuum theory: shear-bands, jamming and dilatancy

S. Luding

*Multi Scale Mechanics, UTwente, POBox 217, 7500AE Enschede, NL**

From molecular dynamics simulations of many atoms or particles, one can extract scalar fields like density or temperature, as well as velocity, i.e. vectorial fields, or tensors like stress, strain, and structure (fabric). Given sufficiently good statistics the data can have a quality that allows to derive constitutive relations about the rheology and flow behavior of complex fluids (like atoms confined in nano-geometry, or granular particle systems) that behave strongly non-Newtonian, with particular relaxation behavior, anisotropy etc. With attractive forces involved, this leads to cohesion added on top of the already non-trivial dynamics of granular matter. Dependent on the energy input (shear-rate), the particles can flow like a fluid, jam and un-jam, or be solid with a very interesting anisotropic structure (contact-and force-networks). The interplay between strain, stress and anisotropy leads to dilatancy and an interesting memory of the packing: the evolution of anisotropy is independent from anisotropy of stress, both in evolution rates as well as in direction, i.e., tensorial eigen-system orientations.

The presentation will show the basic approach to coarse graining following the ideas of Isaac Goldhirsch [3] towards the micro-to-macro transition towards constitutive relations obtained from micro/atomistic/particle simulations. Examples involve the split-bottom ring shear cell and inclined plane avalanche flows.

References

[1] S. Luding, The effect of friction on wide shear bands, Particulate Science and Technology **26(1)**, 33 2008

[2] S. Luding and F. Alonso-Marroquin, The critical-state yield stress (termination locus) of adhesive powders from a single numer. experiment, Granular Matter **13(2)**, 109 2011

[3] I. Goldhirsch. Stress, stress asymmetry and couple stress: from discrete particles to continuous fields. Granular Matter, **12**, 239 2010

*Electronic address: s.luding@utwente.nl