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Hydrodynamic theory of wet particle systems

Modeling, simulation and validation based on microscopic and macroscopic description

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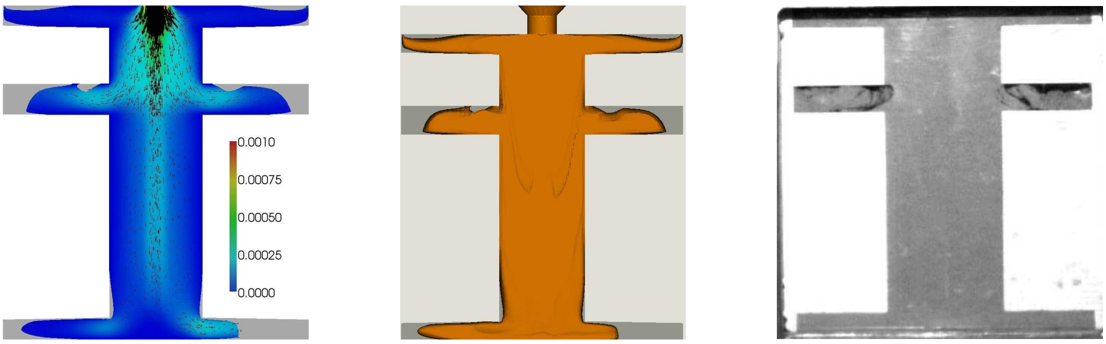
Summary:
The objective of the project is to develop a **hydrodynamic description** of the flow of **wet granular materials**, which is based on detailed knowledge of the links between *micro-scale and macro-scale* material parameters. The main targets of the project are (i) the formulation of suitable *constitutive equations* for the hydrodynamic stress-strain relations, specifically for wet granular materials, (ii) the deduction of the parameters in the constitutive equations from *discrete element simulations*, (iii) the **validation** of the micro-macro transition with data from suitable **experiments** of wet granular materials and (iv) the development of new, more efficient macroscopic *simulation tools* to model realistic, large-scale experiments. As the main working hypothesis, it is assumed that the constitutive **stress-strain relations** can be described by generalized **fluid dynamics** like models, where the parameters of the constitutive model depend on local flow parameters, like e.g. density, pressure, shear rate or volume fractions of the wetting liquid and of the particulate solid phase, respectively.

Example:



(a) granular flow (b) final core (cfd) (c) final core (experiment)

Figure 1: Final state of a core-shooting process, i.e. wet sand form filling, results from CFD simulations (left: velocity, center: contour of the final core) and experiment (right: contour of the final core).

Selection of key publications research group

S. Luding. Cohesive frictional powders: Contact models for tension. *Gran. Matt.*, 10:235, 2008.
S. Luding. The effect of friction on wide shear bands. *Particulate Sci. and Technol.*, 26:3, 2008.
S. Luding and F. Alonso-Marroquin. The critical-state yield stress (termination locus) of adhesive powders from a single numerical experiment. *Granular Matter*, 12:1–11, 2011.

R. Schwarze, A. Rudert, W. Tilch, and J. Bast. Rheological behavior of sand-binder mixtures measured by a coaxial cylinder rheometer. *Int. Foundry Research*, 60:441 – 449, 2008.
A. Rudert, R. Schwarze, J. Bast, and W. Tilch. Computational fluid dynamics of the core shooting process. *International Foundry Research*, 61,3:2 – 9, 2009.
M. Kheiripour Langroudi, S. Turek, A. Ouazzi, and G. I. Tardos. An investigation of frictional and collisional powder flows …. *Powder Technology*, 197:91—101, 2010.
A. Ouazzi, S. Turek, and J. Hron. Finite element methods for the simulation of incompressible powder flow. *Communications in Numerical Methods in Engineering*, 21:581 – 596, 2005.

Goals

Within the project, hydrodynamic models for granular flows with wet contacts shall be developed and validated. The flow rules, which are necessary to close the fundamental conservation laws for mass and momentum, are deduced from DEM simulations by means of micro-macro transition methods. The DEM simulations fit to the flow configurations in a Searl-type granular rheometer. Important effects like dilatancy, which will be found in the DEM simulations, should be retained after the micro-macro transition.

After the implementation of the flow rules into the conservation equations of the fluid flow, the properties of the resulting mathematical model are investigated and, if necessary, problem-specific reformulations are applied before numerical treatment. Then, the mathematical model is implemented into a CFD framework, which allows specific numerical treatment of the resulting nonlinear model equations.

Finally, with the derived CFD models, numerical simulations can be carried out which correspond to the experiments and DEM simulations in the granular rheometer, too. The hydrodynamic models for wet granular flows are this way validated by comparison of results from the CFD simulations and the experiments as well as the (small scale rheometer) simulations. Added, predictive value is then to be expected from the CFD simulations applied to larger scale lab-scale or industrial-scale problems.

Challenges:

Flow rules: There are several proposals for flow rules of dry and wet granular materials available in the literature. These flow rules differ in complexity and in the number of flow parameters, which are combined in the equations. The project uses such a proposal as an initial template (see for instance [A. Rudert et al., 2009; M. Kheiripour Langroudi et al., 2010]), but it is expected that a modified or completely revised version will be necessary to cover all important relations between the flow variables.

Dilatancy: Dilatant behavior is a fundamental component of granular flows (see, for instance, [S. Luding et al., 2011]). However, suitable approximations (like the weak compressibility approximation for Newtonian liquids) for dilatancy must be found for the wet granular flows under investigation in order to allow a hydrodynamic modeling. The relation between anisotropy and dilatancy is not the main subject of this project, but is studied in related research [S. Luding, 2008].

Surface morphology: The surface morphology has an important influence on the flow rules of dry granular materials as evident from DEM simulations [S. Luding, 2008], where parameters like friction or rolling resistance can be easily tuned. In the proposed project, this is also investigated experimentally by using granular materials made of two different basic particles (glass beads and ceramic beads) with similar particle form (spherical) but smooth (glass) or rough surface (ceramic). For all materials we will avoid the artifacts due to mono-disperse sizes by choosing well-defined bi- or poly-disperse size-distributions.

Numerics: The careful formulation of the mathematical model for granular flow shall result in a well-posed problem. Therefore, the final combination of conservation and constitutive equations has to be tested. If ill posed, regularization has to be applied before the numerical treatment. The complex constitutive equations may demand specific numerical techniques for their discretization and hence for their efficient simulation [A. Ouazzi et al, 2005].