Industrial application of continuous powder flow modeling

Goal: Make state-of-the-art continuous powder flow models fit for use by industry and demonstrate to IFPRI members these models can help solve large-scale industrial powder flow problems in reasonable time.

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Installation LAMMPS-Rheo*

0) Set-up Linux system

   windows WSL: *wsl --install -d Ubuntu-22.04*

1) Installation libraries

   https://docs.lammps.org/Howto_wsl.html

   sudo apt install -y cmake build-essential ccache gfortran openmpi-bin libopenmpi-dev libfftw3-dev libjpeg-dev libpng-dev python3-dev python3-pip python3-virtualenv libblas-dev liblapack-dev libhdf5-serial-dev hdf5-tools

   sudo apt install libgsl-dev

2) Downloading LAMMPS-rheo

   git clone -b rheo https://github.com/neocpp89/lammps.git lammps-rheo

3) Adding library to makefile.mpi

   MPI_LIBS = -lgsl

4) Compiling LAMMPS-rheo

   make yes-rheo

   make mpi

   ➔ lmp_mpi executable

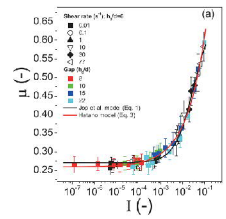
* *Italic-gray* indicated actual code

Running LAMMPS-Rheo

1) Set-up input file in.rheo.sd_silo

   a. Parameters μ(I) rheology model

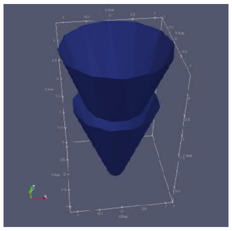
$$\mu(I) = \mu_s + \frac{\mu_2 - \mu_s}{1 + I_0/I}$$



   fix 6 all rheo/stress mu_s 0.271 mu_2 0.68 I_0 0.032

   b. Boundaries of system

   silo.stl



2) Running simulation

   mpirun -np 12 ${PATH}/lmp_mpi < in.rheo.sd_silo

3) Post-processing ➔ silo.dump

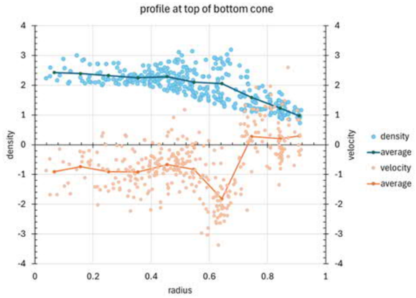
   Paraview 5.12.1 (visuals)

   Python (velocities/forces)

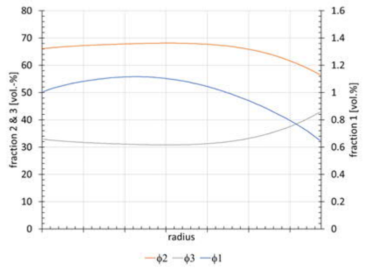
Industrial Applications

1) Flow profile in process equipment

   a. Maldistribution in residence time for double cone above



   b. Adding segregation kinetics (Lueptow) using velocity profile



Application & Scientific Challenges

1) Numerical limits

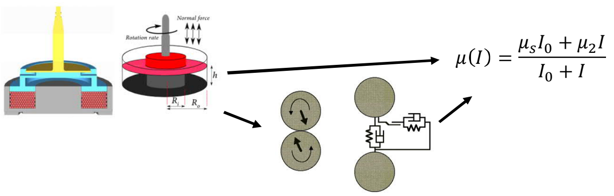
   a. Maximum timestep? $\Delta\tau_c = \frac{\pi r}{\beta(\nu)}\sqrt{\frac{\rho}{G}}$

   b. …

2) Calibration rheology parameter

   a. Directly from experiment to continuous model?

   b. From experiment to DEM to continuous model?



3) Application range & extension rheology model

   a. Industrially encountered deformation rate versus well-posed region

   b. Effect of mixture, cohesion & density variations