Documentation for fluidizedbed case

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1 General

This document describes an *LBDEMcoupling* case simulating a part of a fluidized bed. The bed is considered infinite, which is modelled by using periodic boundary conditions in lateral directions.

2 Running the case

The case is controlled by a set of command line options described in section 4. To run on Lise, a run script is required. This script can be controlled by

submitting shell variables via the command line. An example command line could be

```
qsub -v LD_LIBRARY_PATH=$LD_LIBRARY_PATH,COHESION=0,U_IN=1.2,
   U_MAX_RE=5,OUTDIR=air_test/ run_fluidizedbed.sh
```

The switch $-v$ allows to set variables for access within the script. The script provided will create a subdirectory with velocity and cohesion in the directory name. If this directory already exists, it will be deleted and recreated, thus *be careful what you wish for* when starting a new simulation!

3 Setup

3.1 Geometry

The case consists of a box with extents l_x, l_y, l_z. The x and y directions are fully periodic. In z direction, the bottom wall is a velocity inlet and the top wall is a fixed pressure outlet. Before the outlet, a sponge zone in which the viscosity is gradually increased is added to reduce reflections. At a distance d_{in} form the inlet, a wall is placed. This wall only affects the particles and keeps them from falling into the inlet, which could cause computational trouble.

3.2 Initialization

Prior to a full simulation, a DEM-only initialization procedure is performed. First, the whole domain above d_{in} is filled with particles until a volume fraction of $(1-\epsilon)$[1] is reached. These particles are then allowed to settle under gravity to form a close pack. Thus, setting $(1-\epsilon)$ indirectly controls the height of the un-expanded bed. Directly estimating the bed height is difficult, because other variables (such as the parallelization) also influence particle insertion, but experience has shown that $(1-\epsilon) = 0.4$ results in a bed height of slightly more than a third of the initially filled volume. Once the particles have settled, the real, coupled simulation starts.

[1] ϵ usually denotes the void fraction of a packing, thus $(1-\epsilon)$ is the particle solid fraction

3.3 Run

After the initialization procedure described above, interaction between fluid and solid is switched on, and the simulation is run for t_{max} seconds. Currently, two modes are implemented: constant velocity and ramped velocity. Constant velocity means that the inlet velocity at the bottom of the domain is kept constant at u_{in}^0 for the whole simulation. For ramped velocity, an additonal time t_{ramp} is needed. For $t < t_{ramp}$, the inlet velocity is given by

$$u_{in}(t) = \frac{t}{t_{ramp}} u_{in}^0 \tag{1}$$

and for $t \geq t_{ramp}$ the inlet velocity remains constant.

3.4 Output

The specified output folder must contain subdirectories `tmp/` for LB data and `post/` for DEM data. Data is written at intervals t_{write}. The simulation periodically outputs the flow field (optional) to the LB output directory, and the particle properties to the DEM output directory. Additionally, the averaged pressure is written to a file named `pressure.txt` and the inlet velocity is written to `u\_in.txt`, both in the LB output directory.

4 Command line options

The case accepts parameters via command line options. Unless stated otherwise, these options are all mandatory. All options require a value specified right after their occurence, for example

```
./fluidizedbed -N 8 --u_in 0.5 [other options]
```

All physical quantities are expected in SI units.

- `-N`: controls the resolution of the case. N grid cells per particle diameter will be used.
- `--u_in`: sets the inlet velocity u_{in}^0

- `--u_max_lb`: sets the maximum LB velocity $u_{max,lb}$. Decreasing $u_{max,lb}$ decreases the time step and can increase stability in some cases. For this case, a value of $u_{lb,max} = 0.05$ has been found to work just fine.

- `--dt_dem_max`: sets an upper limit for the DEM time step. The actual time step depends on the exact value of the LB time step and is computed internally.

- `--outdir`: specifies the directory to which the output is written. This directory must exist, and contain two subdirectories named `tmp/` for LB data and `post/` for DEM data.

- `--rho_f`: controls the fluid density ρ_f.

- `--nu_f`: controls the kinematic viscosity of the fluid ν_f.

- `--rho_s`: controls the bulk density of the particles ρ_s.

- `--radius`: sets the radius r_s of the particles.

- `--vol_frac`: sets the particle volume fraction $(1 - \epsilon)$ of the initial packing. This indirectly controls the height of the particle bed, and should not be much higher than 0.4.

- `--lx`, `--ly`, `--lz` set the size of the simulation box. The full resolution per direction is then given by $N_{tot,xyz} = N\frac{l_{xyz}}{2r_s}$.

- `--inlet_distance`: The distance d_{in} of the wall holding the particles to the inlet at $z = 0$.

- `--max_t`: the runtime of the simulation, t_{max}.

- `--write_t`: the interval at which data is written, t_{write}.

- `--write_flowfield`: controls if the full flow field is written to disk (the data can be quite large). Accepts anything that can be casted to `bool`, such as `true`/`false`, 0/1, ... *This argument is optional, default setting is* `false`.

- `--ramp_time`: The time to ramp up the inlet velocity to the final value set by `--u_in`, t_{ramp}. Set to zero (or leave out alltogether) to disable ramping. *This argument is optional, default is no ramping.*

- `--cohesion_energy_density`: Cohesion energy density. The case uses the sjkr cohesion model of LIGGGHTS, and the reader is referred to the LIGGGHTS documentation for details on the cohesion model.

- `--use_smagorinsky`: controls whether Smagorinsky-style turbulence modelling is used. Needs a boolean value just as `--write_flowfield`. *This argument is optional. Default is* `false`.

- `--c_smago`: if the Smagorinsky model is used, the Smagorinsky "constant" c_s is set. *This argument is optional. Default value is* $c_s = 0.15$.