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Influence of coarse-graining parameters on the analysis of DEM simulations of silo flow

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Abstract

10 The discrete element method (DEM) is used extensively for the simulation of granular materials and in powder technology. Averaging or coarse graining (CG) techniques, also referred to as the micro-macro transition, are applied to the particle data from DEM simulations to extract bulk continuum fields such as density, velocity and stress, which are important for the design of
15 a great majority of engineering applications. Although numerous papers have been published on such CG techniques, there still remain considerable challenges, chiefly because both the spatial and the temporal scales vary between different engineering processes.

The major aim of this paper is to answer the question of what temporal
20 and spatial averaging scales should be adopted, and what is their influence on the micro-macro projected continuum fields. A model silo with a non-steady, inhomogeneous internal flow pattern is used as a test case, where three distinct flow regimes are present, *i.e.* : (i) a stagnant zone, (ii) a high

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shear localisation zone and (iii) a core zone with fast flow. The spatial and
25 temporal scales are varied systematically and display interesting relationships
with other model parameters such as the sampling frequency and simulation
time; however, there is a range (plateau) of spatial and temporal scales which
provide continuum fields independent on the coarse-graining width and time
scales.

30 Then we compare several ways to identify/locate the shear band centre
and width. Based on the (simple-shear) strain rate (horizontal gradient of
vertical velocity), the shear band is best defined, together with a fitting
procedure that allows to smoothly find its centre and width. The other
continuum fields are analysed, showing a strongly anisotropic stress tensor,
35 with an arch of higher horizontal stresses observed in the central region, while
the stress in the stagnant zone transfers the weight of the flow to the walls
and the base plate. In the sheared and fast-flowing zones, the shear
stress is predicted by the $\mu(I)$ -rheology, but this has to be based on the
objective (complete tensorial) strain-rate, since the flow and shear geometry
40 are not aligned along one direction. Further non-Newtonian mechanisms can
be observed, but are not detailed in this study.

Keywords: Coarse graining, granular systems, DEM, homogenisation

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1. Introduction

Granular systems – conglomerations of individual particles – are ubiqui-
45 tous in both industry and nature. Granular materials range from sand, sugar,
coffee, rice and iron-ore to man-made conglomerates such as tablets or cap-
sules. An understanding of the dynamical behaviours of granular media is of

paramount importance to the pharmaceutical, mining and food processing industries, and highly relevant also to the prediction and prevention of land-
50 slides, earthquakes and other geophysical phenomena. The Discrete Element Method (DEM) is a powerful computational tool to study such systems; the method allows the simulation of tens of millions of individual particles by solving Newton’s laws for each particle. To visualise and analyse the granular system, local macroscopic quantities such as density, velocity and stress
55 can be extracted from the discrete simulation data (particle positions and velocities, interaction forces and torques).

Several micro-macro transition techniques have been developed to calculate continuum fields, as shown in [1]. Particularly the stress tensor is of interest: the techniques include the Irvin-Kirkwood approach [2, 3], which
60 allows the calculation of the stress tensor within small volumes or bins, or the method of planes [4]. Here, we use the coarse-graining approach (CG) as described in [5, 6]. The comparison between the latter two approaches can be found in [7].

The CG method [5, 6] has several advantages over other methods, including: *i)* the fields automatically satisfy the conservation equations of contin-
65 uum mechanics, even for single particles (no ensemble averaging is required), and *ii)* it is not assumed that the particles are rigid or spherical. The only assumptions are: each contact between particles is assumed to be a point contact, and collisions are not instantaneous. CG has been successfully applied
70 to granular flows, for experimental [8, 9] and simulational data [10, 11, 12], as well as molecular flows [13].

Note that the word ‘coarse-graining’ is ambiguous: In molecular dy-

namics, coarse-graining consists of replacing an atomistic description of a molecule with a lower-resolution coarse-grained model that averages over the
75 fine details. It is also used as a synonym for homogenisation methods or the micro-macro transition. Here, we apply it to the specific micro-macro transition method developed in [5, 6].

Coarse-graining involves a spatial scale, w , which determines the extent of the volume contributing to the field data at each point. When temporal
80 coarse-graining is applied as well, one also needs a temporal scale, Δt . These two scales have to be chosen carefully: for very small scales, the amount of data at each point is so small that the resulting fields can strongly fluctuate; for very large scales, the fields are scale-dependent due to the ‘smearing-out’ of macroscopic gradients. For a range of scales w and Δt (and a sufficient
85 amount of data), however, the field values plateau, *i.e.* are scale-independent [14].

The spatial CG scale was studied in detail in [15] for steady granular chute flows. Two distinct coarse-graining length scale ranges were identified in terms of the particle diameter d , where the fields are almost w -independent.
90 The smaller, sub-particle length scale, $w \ll d$, resolves details on the particle scale, such as density and shear rate oscillations between particle layers. The larger, particle scale, $w \approx d$, leads to bulk stress, velocity, and density fields in which particle-scale effects are averaged out, and is thus appropriate to study the macroscopic behaviour. However these findings only apply to
95 steady state flow condition and may not be valid for other conditions, as studied here.

Spatial coarse-graining, however, is often not sufficient to obtain well-

defined macroscopic fields, as the fields can show strong fluctuations over time: In these cases, temporal coarse-graining is applied, usually by averaging the data over a time interval Δt . While Δt can be arbitrarily large in steady situations, it is unclear how to choose the temporal scale in dynamic situations.

In this study, the coarse-graining (CG) technique is applied to a silo flow model with internally varying flow patterns. We begin by reviewing the spatial coarse-graining approach in §2, extending it to non-spherical particles. Then the silo flow model is introduced in §3. In §4, CG is applied to the silo flow and the resulting fields are used to define the flow regions and determine the flow rheology in the shear band.

2. Coarse-graining methodology

To extract the macroscopic fields, we use the spatial coarse-graining approach as detailed in Weinhart *et al.* [10, 16] and references therein, which will be reviewed in this section.

It is assumed that collisions are not instantaneous, that each particle pair, has a finite amount of contacts, and that each contact area is small enough that it can be replaced by a single contact point. The evolution of the system is described by evaluating Newton's law of motion, where the force $\vec{f}_i$ and torque $\vec{t}_i$ acting on particle i is given by the body force $\vec{f}_i^b$ and the interaction forces $\vec{f}_{ij}^k$ and torques $\vec{t}_{ij}^k$ with other particles and walls,

$$\vec{f}_i = \vec{f}_i^b + \sum_{j=1}^{N+N_b} \sum_{k=1}^{C_{ij}} \vec{f}_{ij}^k, \quad \vec{t}_i = \sum_{j=1}^{N+N_b} \sum_{k=1}^{C_{ij}} \vec{t}_{ij}^k + (\vec{c}_{ij}^k - \vec{r}_i) \times \vec{f}_{ij}^k. \quad (1)$$

Here, particles are labeled from 1 to N , walls are labeled from $N + 1$ to

$N + N_b$, contacts between particles i and j are labeled from 1 to C_{ij} , $\vec{r}_i$ is the
115 centre of mass of particle i , and $\vec{c}_{ij}^k$ is the contact point between particles i
and j .

[Figure 1 about here.]

2.1. Mass density and velocity

In statistical mechanics, it is assumed that each particle's mass is located at its centre $\mathbf{r}_i$ (i.e. not distributed within the particle volume). Thus, the microscopic (point) mass density, ρ^{mic} , at a point $\mathbf{r}$ at time t is defined by

$$\rho^{\text{mic}}(\mathbf{r}, t) = \sum_{i=1}^N m \delta(\mathbf{r} - \mathbf{r}_i(t)), \quad (2)$$

where $\delta(\mathbf{r})$ is the Dirac delta function.

A macroscopic mass density field can then be extracted by convoluting the microscopic mass density with a coarse-graining function $\mathcal{W}(\mathbf{r})$, which yields

$$\rho(\mathbf{r}, t) = \int_{\mathbb{R}^D} \rho^{\text{mic}}(\mathbf{r}', t) \mathcal{W}(\mathbf{r}') d\mathbf{r}' = \sum_{i=1}^N m \mathcal{W}(\mathbf{r} - \mathbf{r}_i(t)), \quad (3)$$

120 with D the number of spatial dimensions.

A cut-off Gaussian coarse-graining function is used,

$$\mathcal{W}(\mathbf{r}) = V_\omega^{-1} \exp\left(-\frac{r^2}{2\omega^2}\right), \text{ if } r := |\mathbf{r}| < c, \text{ 0 else,} \quad (4)$$

with coarse-graining width $w > 0$ and cutoff $c = 3w$. The normalisation constant V_ω is chosen such that the integral over the coarse-graining function

is unity,¹

$$\int_{\mathbb{R}^D} \mathcal{W}(\mathbf{r}) \, d\mathbf{r} = 1, \quad (5)$$

which is required such that the integral over the density equals the total mass.

The Gaussian function is chosen as it delivers smooth results; the cut-off is applied to limit the computational expense. However, other coarse-graining functions are possible, such as Heaviside or Lucy polynomials (see figure 1), as long as they satisfy equation (5). The resulting coarse-grained fields depend only weakly on the choice of coarse-graining function. Instead, the standard deviation of the coarse graining function, $\sigma_\omega \approx \sqrt{D}w$, turns out to be the key parameter [6, 17, 15].

Similarly, the coarse-grained momentum density vector $\mathbf{p}(\mathbf{r}, t)$ is given by

$$\mathbf{p}(\mathbf{r}, t) = \sum_{i=1}^N m \mathbf{v}_i \mathcal{W}(\mathbf{r} - \mathbf{r}_i), \quad (6)$$

where $\mathbf{v}_i$ is the velocity of particle i . The macroscopic velocity field $\mathbf{V}(\mathbf{r}, t)$ is then defined as the ratio of momentum density and mass density fields,

$$\mathbf{V}(\mathbf{r}, t) = \mathbf{p}(\mathbf{r}, t) / \rho(\mathbf{r}, t). \quad (7)$$

2.2. Stress

Next, we consider the momentum conservation equation with the aim of establishing the macroscopic stress field, $\sigma_{\alpha\beta}$. We split the stress

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^k + \boldsymbol{\sigma}^c, \quad (8a)$$

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¹For three spatial dimensions, $V_\omega = \text{erf}(\frac{c}{\sqrt{2}w}) - \sqrt{\frac{2}{\pi}} \frac{c}{w} \exp(\frac{-c^2}{2w^2})$, and the standard deviation is approximately $\sigma_\omega \approx \sqrt{3}w$.

into its kinetic ($\boldsymbol{\sigma}^k$) and contact ($\boldsymbol{\sigma}^c$) contributions

$$\boldsymbol{\sigma}^k = \sum_{i=1}^N m \mathbf{V}'_i \mathbf{V}'_i \mathcal{W}(\mathbf{r} - \mathbf{r}_i), \quad (8b)$$

$$\boldsymbol{\sigma}^c = \sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^{N+N_b} \sum_{k=1}^{C_{ij}} \mathbf{f}_{ij} \mathbf{a}_{ij}^k \int_0^1 \mathcal{W}(\mathbf{r} - \mathbf{r}_i + s \mathbf{a}_{ij}^k) ds \quad (8c)$$

with interaction forces, $\mathbf{f}_{ij}^k = -\mathbf{f}_{ji}^k$, and branch vectors, $\mathbf{a}_{ik} = \mathbf{r}_i - \mathbf{c}_{ij}^k$, from the contact point $\mathbf{c}_{ij}^k$ to the particle's centre of mass $\vec{r}_i$. Furthermore, the boundary interaction force density is introduced

$$\mathbf{t} = \sum_{i=1}^N \sum_{j=N+1}^{N+N_b} \sum_{k=1}^{C_{ij}} \mathbf{f}_{ji}^k \mathcal{W}(\mathbf{r} - \mathbf{c}_{ij}^k), \quad (9)$$

which is a measure of the force the particles exert on the wall and has nonzero values only near the walls [16].

While the density, momentum density and contact stress are scale-independent on the particle scale, $w \approx d$, this is not true for the fluctuation velocity field [18],

$$\mathbf{V}'_i(\mathbf{r}, t) = \mathbf{v}_i(t) - \mathbf{V}(\mathbf{r}, t). \quad (10)$$

Instead, the fluctuation velocity (and consequently the kinetic stress) is only
135 scale-independent for small spatial scales, $w \leq 0.1d$, as shown in [15]. We refer the interested reader to Artoni and Richard [19], who developed a scale-independent definition of the fluctuation velocity by splitting the kinetic stress into a scale-dependent component reflecting affine deformations and a scale-independent component attributed to fluctuation velocities.

By design [6, 16], these newly defined local macroscopic fields satisfy

exactly the continuity and momentum equations

$$\partial_t \rho + \nabla \cdot \rho \vec{\mathbf{V}} = 0, \quad (11a)$$

$$\partial_t(\rho \mathbf{V}) + \nabla \cdot (\rho \mathbf{V} \mathbf{V}) = \nabla \cdot \boldsymbol{\sigma} + \rho g - \mathbf{t}. \quad (11b)$$

140 where the short-hand notation $\partial_t = \partial/\partial t$ is used. The definitions for density, momentum density and stress were derived in [6, 16] assuming a single contact point between each particle pair i, j ; however, the extension to a finite number of contact points is straightforward.

2.3. Averaging over time and spatial dimensions

Further, time-averaging can be applied to decrease temporal fluctuations. For that, a uniform distribution function is used,

$$\langle \rho \rangle_t = \frac{1}{\Delta t} \int_{t-\Delta t/2}^{t+\Delta t/2} \rho(\mathbf{r}, t) dt. \quad (12)$$

145 In steady situations, the fields are homogeneous (*i.e.* ‘unvarying’) in time and thus the time averaging interval Δt can be arbitrarily large. For unsteady situations, however, the average value becomes scale-dependent, and time averaging can only be applied over a sufficiently small interval, as we will investigate further in this paper.

Similarly, the continuum fields can be averaged over those spatial directions in which the flow is homogeneous (in this case, the thickness y). This will be denoted by angled brackets; *e.g.*, the average of ρ over the y -direction is given by

$$\langle \rho \rangle_y(x, z, t) = \frac{1}{y_1 - y_0} \int_{\mathbb{R}} \rho(\mathbf{r}, t) dy, \quad (13)$$

where $[y_0, y_1] = [0, 4]\text{cm}$ denotes the size of the domain. The integration is applied over the whole domain to capture the tails of the CG functions, which

sometimes extend beyond the domain. To save computational effort and to accurately resolve the integral, this averaging is done analytically, *i.e.* by using an analytic expression for the integral of the coarse graining function, $\langle \mathcal{W} \rangle_y(x - x_i, z - z_i, t) = \int_{\mathbb{R}} \mathcal{W}(\mathbf{r} - \mathbf{r}_i, t) dy$, resulting in the expression

$$\langle \rho \rangle_y(x, z, t) = \sum_{i=1}^N m_i \langle \mathcal{W} \rangle_y(x - x_i, z - z_i, t). \quad (14)$$

The averaged velocity is then evaluated as

$$\langle \mathbf{V} \rangle_y = \langle \mathbf{p} \rangle_y / \langle \rho \rangle_y. \quad (15)$$

150 The averaged fields still satisfy the mass and momentum equations, if the averaging is applied in directions where the flow is homogeneous.

3. DEM modelling of silo flow

Over the last decades, DEM has been used to model many granular flow situations involving complex flow patterns that evolve spatially and tem-
 155 porally. In this type of problems, spatial and temporal averaging take an important role in the analysis of the results. Here a DEM model of flow from a flat-bottomed silo has been specifically chosen to study the influence of the spatial and temporal coarse-graining parameters. With a central outlet through the flat bottom, an internal flow channel develops and evolves over
 160 time providing a rich phenomenological and fundamental benchmark case.

The flow consists of three distinct zones: A stagnant zone near the side walls, a zone with high localized shear and a fast core flow zone in the middle of the silo.

The geometry of the silo model is presented in Figure 2. Periodic bound-
165 ary conditions are applied in y -direction, such that the flow is homogeneous
in y .

[Figure 2 about here.]

The model considers 56 241 non-spherical monodisperse particles. Each
particle is created with two overlapping spheres [20] with centre-centre dis-
170 tance $0.25d_s$, where $d_s = 3\text{ mm}$ is the diameter of the constituent spheres, as
shown in Figure 3. For the purpose of the present study, the particle size d
is defined as the diameter of the volume-equivalent sphere ($d = 3.33\text{ mm}$).

[Figure 3 about here.]

The Hertz-Mindlin contact model implemented in EDEM® [21] is used,
175 with the material properties of the particles: mass density of 950 kg/m^3 ;
shear modulus of 0.1 GPa ; Poisson's ratio 0.4 . The material properties of the
walls are: shear modulus 10 GPa and Poisson's ratio 0.2 . The contact model
parameters for the particle-particle interaction considers a friction coefficient
of 0.577 ; for the particle-wall interaction a friction coefficient of 0.5 is used.
180 The coefficient of restitution is set to 10^{-4} , but does not have influence in
the flow patterns. The Relative Velocity Dependent (RVD) rolling friction
model [22] is used with a rolling friction coefficient of 0.2 . We integrate the
resulting force and torques in time using the Velocity-Verlet algorithm with
a time step of $1.54\text{ }\mu\text{s}$. The total simulation time is 2.5 s , and a sampling
185 frequency of 200 Hz is used to obtain the continuum fields.

4. Results

Static, sheared, and fast-flowing zones: Figure 4 shows the evolution of the particle flow in the silo. The particles are stationary as long as the outlet is closed, *i.e.* $t < 0.1$ s. After the outlet is opened, particles begin to flow out
190 as flow regime begins to propagate upwards and a nearly steady flow begins to develop in the centre of the silo; the outflow rate is steady for $t > 0.6$ s. The particles near the side walls remain static; this static zone slowly decreases in size as the silo is emptied. To study the typical flow behaviour, we investigate the flow at $t = 1.2$ s, where the flow is fully developed and 2/3 of the initial
195 particles still remain in the silo.

[Figure 4 about here.]

We can clearly distinguish three zones: *(i)* a stagnant zone near the side and bottom wall, *(ii)* a zone of high shear localization, and *(iii)* a fast-flowing core. To study these zones further, we select three points at horizontal
200 positions $x_0 = 0$ cm, $x_1 = -3.75$ cm $\approx 11d$, $x_2 = -6.25$ cm $\approx 19d$ and at height $z = 10$ cm $\approx 30d$, one from each zone, to be investigated in detail (see figure 4).

4.1. Averaging over the depth y

Next, we average over the directions, in which the macroscopic fields
205 are homogeneous. This is the case in the y -direction, in which the domain is periodic and uniform. We observe that the variations of solid fraction, momentum density and stress in the y -direction are smaller than the standard deviation (not shown). Thus, all results shown here are averaged over the y -direction.

210 4.2. Homogeneity in time

To determine an appropriate averaging time interval $[t - \frac{\Delta t}{2}, t + \frac{\Delta t}{2}]$, we plot the profiles of the instantaneous solid fraction, momentum density and downward stress over time at x_0 , x_1 , and x_2 in Figure 5. After the silo exit is opened, the momentum density in the core flow zone increases sharply before
 215 dropping back to level off at a nearly constant value. This is associated with a dilation of the solid, resulting in a rapid drop of the local solid fraction before recovering to level off at a solid fraction of $\nu \approx 0.5$. There is a corresponding increase in vertical stress in the surrounding stagnant zone as the vertical stress drops to zero in the core flow zone.

220 After the velocity has levelled off ($0.75 \text{ s} < t < 2 \text{ s}$), all profiles are nearly constant in time in the flowing core (x_0) and the shear zone (x_1). In the static zone (x_2), the stress decreases over time, as the silo is emptied, whereas the shear zone displays mostly constant behaviour throughout.

[Figure 5 about here.]

225 In figure 6, the dependence on Δt of the averaged solid fraction, momentum density and downward stress is presented. The averaged variables in the figures present stable values for the stagnant and flowing zones for Δt of up to 1.5s. However, the shear zone presents a degree of variation especially for the solid fraction, with a lower variation with $\Delta t < 1 \text{ s}$ and increasing for
 230 higher values of Δt . This can be explained by the displacement of the shear band during the discharge. For large values of Δt , the spatial average in the shear zone (x_1) captures particles outside the shear band, where the solid fraction is higher. The same occurs within the stagnant zone (x_2), where part of the shear band and the initial conditions is captured for $t > 1.8 \text{ s}$.

[Figure 6 about here.]

The variation for high values of Δt can be observed in a better way using the coefficient of variation (CV) of the averaged variables, as presented in figure 7. Except for the stress in the static zone, which decreases over time, the CV of all variables increases gradually until $\Delta t = 0.5$ s, then is nearly
 240 stable for $0.5 \text{ s} < \Delta t \leq 1.1 \text{ s}$. For higher Δt s, the CV of the averaged variables increases, as we average over an interval that includes a significant share of non-steady flow, which occurs before $t < 0.75$ s. For $\Delta t \leq 1.1$ s, the CV of solid fraction is negligible (< 0.02), as it does not vary strongly in time. The CV of momentum density is larger, but varies within a narrow range (~ 0.1
 245 in the flowing zone and ~ 0.2 at the shear and static zones), and the same holds for the stress in the flowing and shear zone (~ 0.4). In the stagnant zone, however the CV of stress (and solid fraction) show a gradual increase for $\Delta t > 0.5$, as these variables strongly vary within this interval, as shown in figure 5. This means the chosen time interval should be smaller than 0.5 s.

250 To select the time interval, the interplay with the coarse-graining width (w) must be considered. In the following section the dependence between both parameters is analysed.

[Figure 7 about here.]

4.3. *Dependence on the coarse-graining width*

255 In order to obtain an accurate representation of the coarse-grained variables, appropriate choices for the time-averaging interval and the coarse-graining width are required. To determine the appropriate coarse-graining

width we plot the comparison of the spatio-temporally averaged solid fraction (figure 8), momentum density (figure 9) and downward stress (figure 10) for the three sample points with different values of the coarse-graining width and time intervals.

In figure 8 an important influence of Δt and w in the solid fraction is found for $w/d < 0.5$, where the computed solid fraction depends on the chosen temporal and spatial scales. For $w/d > 1.5$, the solid fraction diverges in the stagnant and shear zone. For the flowing core, the time averaged and instantaneous solid fraction differs for low values of w/d , but converges to a stable value for $w/d \geq 1.5$.

[Figure 8 about here.]

A similar influence of w/d is found for the momentum density (figure 9). In this case the influence on the time interval is higher, particularly in the flowing (x_0) and shear (x_1) zones. A noticeable exception is again the instantaneous case ($\Delta t = 0$) which deviates significantly from the others.

[Figure 9 about here.]

For the stress (figure 10), a clear plateau is found between $0.5 < w/d < 1.0$ for the stagnant zone (x_2), where a low influence of Δt is seen. For the flowing core (x_0) and shear zone (x_1), the influence of Δt is not significant for $w/d > 0.5$, whilst a high variation of the value with w is found. This contrasts with the relatively stable solid fraction with the temporal and spatial scales, revealing the nature of the problem that whilst solid friction may remain

relatively constant in the shear and core flowing zones in a silo, the stress regimes can vary much more. Again the instantaneous case ($\Delta t = 0$) deviates significantly from the others which suggests that computing DEM results using an instantaneous snapshot can lead to erroneous result.

285

[Figure 10 about here.]

Based in the previous results, the range of $0.5 < w/d < 1.5$ appears to be the most favourable w/d values to use. Similar plateaus in the coarse-graining width w/d have been observed in [23, 14, 15, 24], as discussed in the introduction. Thus, the coarse-grained fields appear to be scale-independent
 290 for $w = d$ in the flow regimes studied. For this spatial scale, it was shown in §4.2 that time-averaging shows that the variables are independent of the chosen time interval for $\Delta t < 1.2$ s. However, the variance of the time-dependent stress in the stagnant zone increases for $\Delta t > 0.4$ s (figure 7). Therefore $\Delta t = 0.4$ s is selected as the optimal time-averaging interval for
 295 this problem.

After the temporal and spatial averaging parameters are thus chosen, the coarse-graining technique is used to study the flow pattern in the model as presented in the following sections.

4.4. Shear band study

300

Three zones: First, we study the profiles of solid fraction (packing density), velocity, and shear rate, plotted in figure 11. The fields are averaged in depth y and over a small time interval $1 \text{ s} < t < 1.4 \text{ s}$ and a coarse-graining width of $w = d$ is used, as justified above. A resolution of 100×60 points in x and z is chosen to resolve the data spatially. We can clearly distinguish

305 some key features of the three zones: *(i)* a stagnant zone near the side and bottom walls, where the density is high, the velocity nearly vanishes, and the stress increases with height, as expected from a hydrostatic stress profile (figure 16); *(ii)* a zone of high shear localization, combined with a low density (due to dilatancy) and moderately large stresses; and *(iii)* a fast flowing core,
 310 in which the velocity is high, but with small shear rates and lower stresses.

[Figure 11 about here.]

[Figure 12 about here.]

Shear band: In order to study the shear band in more detail, *i.e.* the zone between the static and the flowing region of the granulate, we attempt to define the location of its centre and width. Three simple methodologies are proposed to define the location of the shear band (Figure 12), using (a) the *tensorial* shear rate $\dot{\gamma} = \frac{1}{2} \sqrt{(\partial_x v_z + \partial_z v_x)^2 + (\partial_x v_x - \partial_z v_z)^2}$, (b) the horizontal gradient of vertical velocity $\partial_x v_z$, and (c) the inertial number $I = \frac{\dot{\gamma} d}{\sqrt{p/\rho_p}}$, which is the tensorial shear rate scaled by a combination of pressure p , particle size d and density ρ_p that represents the response time-scale of the material. As the shear rate is rapidly decreasing in height, we normalise each quantity f by its maximum at each height z , which is denoted by the hat operator,

$$\hat{f}(x, z) := \frac{f(x, z)}{\max_x f(x, z)}. \quad (16)$$

While the tensorial shear rate definition is sensitive to both pure and simple shear, the horizontal gradient of vertical velocity does not take pure shear
 315 contributions into account. Both definitions show non-zero values in the shear band (where simple shear is active), but the horizontal gradient of

vertical velocity vanishes in the lower part of the fast-flowing core: here, the flow is accelerated, causing a vertical extension, and the width of the core region contracts towards the orifice, causing pure shear.

320 At first, we define the location of the left and right shear bands, $C_l(z)$ and $C_r(z)$, by the maxima of each quantity in the left ($x \leq 0$) and right half ($x \geq 0$) of the domain; the resulting shear band locations are similar for all three definitions. Next, we define the width of the shear band as all values for which each scaled quantity is larger than a given tolerance τ , which we
 325 choose here to be 0.6 (with 1 being the maximum), shown demarcated by the solid lines in figure 12.

We see clear differences between the three definitions: The scaled horizontal gradient of vertical velocity is only larger than $\tau = 0.6$ in a tight region around the centre of the shear band, giving a good definition of the
 330 shear band throughout the silo. This is also true for the tensorial shear rate; however, the large values in the lower region of the flowing zone decreases the quality of the shear band definition. This undesired effect is intensified if we consider the inertial number, as the pressure p in the lower flowing zone is much lower than in the shear band, thus increasing the inertial number
 335 there. Therefore we choose to use $\partial_x v_z$ for the shear band definition.

[Figure 13 about here.]

[Figure 14 about here.]

Defining the shear band centre as the location of the maximum (figure 12) has two disadvantages: Firstly, as the grid resolution is finite (100 points in x -direction), the centre of the shear band can only be located with an accuracy

of 0.15 cm, resulting in an undesirable stepwise definition. Secondly, the shear band splits into several arms for small w , as the larger noise in the data can create local maxima of the shear rate far from the shear band, see figure 13. To avoid these effects, two other definitions were tested, as shown in figure 15: Firstly, the centres and widths of the shear bands are defined as the centroids and the hygroscopic radius in the left and right half plane, respectively, with $\partial_x v_z$ acting as the mass,

$$C_l(z) = \frac{\int_{x_0}^0 \partial_x v_z x dx}{\int_{x_0}^0 \partial_x v_z dx}, \quad W_l(z) = \sqrt{\frac{\int_{x_0}^0 \partial_x v_z (x - C_l)^2 dx}{\int_{x_0}^0 \partial_x v_z dx}}, \quad (17a)$$

$$C_r(z) = \frac{\int_0^{x_1} \partial_x v_z x dx}{\int_0^{x_1} \partial_x v_z dx}, \quad W_r(z) = \sqrt{\frac{\int_0^{x_1} \partial_x v_z (x - C_r)^2 dx}{\int_0^{x_1} \partial_x v_z dx}}. \quad (17b)$$

This produces a smooth definition of the shear band. The centre of the shear band, however, is badly approximated by the centroid definition, as
 340 the actual shear band is asymmetric, with the peak shear rate close to the outer boundary of the shear band. Therefore, a second fit was obtained by only considering values for which $\widehat{\partial_x v_z}$ is above a tolerance of $\tau = 0.6$, producing a good approximation of the shear band; however, the width of the shear band is now dependent on the choice of τ .

Therefore, a fourth definition of the shear band was chosen, where the centre and width of the shear band were defined by fitting $\partial_x v_z$ by a Gaussian function with the least squares approximation

$$\min_{C_l, W_l, M_l} \int_{x \leq 0 \cap \widehat{\partial_x v_z} > \tau} \left| \partial_x v_z(x, z) - M_l \exp \left(-\frac{(x - C_l)^2}{2W_l^2} \right) \right|^2 dx \quad (18a)$$

$$\min_{C_r, W_r, M_r} \int_{x \geq 0 \cap \widehat{\partial_x v_z} > \tau} \left| \partial_x v_z(x, z) - M_r \exp \left(-\frac{(x - C_r)^2}{2W_r^2} \right) \right|^2 dx, \quad (18b)$$

345 As the shear band is not symmetric, we again only consider values for which $\widehat{\partial_x v_z} > \tau$; for this definition, however, the shear band width *is independent of the choice of τ for $\tau > 0.5$.*

To show that the shear band is now well-defined, the centre and width location of the shear band is plotted for varying coarse-graining widths w in figure 14. We observe that the both the shear band centre and band width
 350 are nearly stable for $0.2 < w/d < 2$, with the centre of the band moving slightly away from the central axis as w decreases, probably because of a varying shear gradient in the region.

4.5. Stress analysis

355 *Stress anisotropy:* To study the stress across the flow regimes over time, we plot the normal stresses as well as the shear stress σ_{xz} in figure 16. This represents the complete description of the stress, as the remaining shear stress components are fluctuating around zero and the stress tensor is nearly symmetric. We observe that the normal stress components differ strongly from each other, with the stress in downward direction, σ_{zz} , being highest
 360 and the lateral stress, σ_{xx} the weakest. The stresses in the static zone are the highest stresses and increase with depth, which indicates that they are governed by the weight of the solid and the friction on the wall. An arch of higher normal stress σ_{xx} extends through the flowing zone from the top of the static zone (best seen in the σ_{xx} plot in figure 16), thus allowing the flow
 365 below the arch to flow at lower pressure.

[Figure 15 about here.]

Stress balance: If we average the third momentum balance equation (11b)

over x , y and $t \in [1, 1.4]$ s and assume that the rate of change in momentum density is negligible, we obtain a balance between the weight of the flow, the downward normal stress and the force acting on the walls,

$$g_z \langle \rho \rangle_{xyt} = -\partial_z \langle \sigma_{zz} \rho \rangle_{xyt} - \langle t_z \rangle_{xyt}. \quad (19)$$

This is shown to be valid in Figure 17. To better understand the wall interaction force density, $\mathbf{t}$ is split into three components $\mathbf{t} = \mathbf{t}^l + \mathbf{t}^r + \mathbf{t}^b$, which denote the forces on the left and right side wall and the bottom wall, respectively. The ratio of shear to normal forces acting on the side walls (i.e. the side wall friction) is nearly independent of height (except at the lowest heights, $z < 3$ cm, where the shear stress vanishes), with a mean value of $|t_x|/|t_z| = 0.41$ at the left and $|t_z|/|t_x| = 0.42$ at the right side wall. Thus, the amount of gravitational force balanced by shear stress on the side walls is given by the side wall friction multiplied by the pressure acting on the side wall. We obtain that $(t_z^l + t_z^r)/t_z = 21\%$ of the flow weight is held by the shear forces on the side walls, while $t_z^b/t_z = 79\%$ is held by the downward stress, which is then transferred to the base wall.

[Figure 16 about here.]

4.6. Flow rheology

Next, we take a look at the objective, mobilised macroscopic friction as defined and studied in [15]. It is defined as the ratio between shear stress and normal stress,

$$\mu = \frac{1}{\sqrt{6}p} \sqrt{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2}, \quad (20)$$

where σ_i denotes the eigenvalues of the stress tensor and p the pressure. The macroscopic friction ranges from 0.7 to nearly 1 almost everywhere except near the bulk surface, as shown in Figure 18a; the large value is consistent with the chosen shape, microscopic interparticle sliding, and rolling friction. It is particularly high in the shear zone, as shown in Figure 18b, which is not surprising, as the friction in sheared (critical) flows is known to be a function of the inertial number, $I = \frac{\dot{\gamma}d}{\sqrt{p\rho_p}}$. While no clear functional behaviour can be seen for low inertial numbers, the friction is clearly increasing with inertial number. This is in agreement with the results of [25, 26, 27, 28]; a more detailed rheological study is planned in a future publication.

[Figure 17 about here.]

5. Summary and conclusions

In this article, coarse-graining (CG) formulations (i.e. the micro-macro transition) are reviewed and applied to a simulation of the flow through a model scale quasi-2D silo, as an example of a spatially and temporally inhomogeneous system. The system is homogeneous in depth y and, consequently, all variables are averaged over this direction. The remaining two-dimensional fields show three well defined regions, where a fast-flowing core is separated by a narrow shear band from a stagnant outer region. The temporal evolution of the system shows that the flow is fully developed in the interval $0.75\text{ s} < t < 2\text{ s}$, where most fields vary little over time except that the stresses decreases gradually over time due to the decreasing height of the solid.

405 The CG formulation depends on two parameters, the spatial and temporal averaging length scales w and Δt . To determine the optimal parameters, one point from each region is analysed for different parameter values. Time-averaging around the instant $t = 1.2$ s shows that the variables are independent of the chosen time interval for $\Delta t < 1.2$ s. However, the variance of
 410 the (time-dependent) stress in the stagnant zone increases considerably for $\Delta t > 0.4$ s; therefore, $\Delta t = 0.4$ s is selected as the optimal time-averaging interval.

The results for the coarse-graining width w show that for $w/d < 0.5$, the averaged fields are strongly dependent on the choice of Δt for $\Delta t < 0.4$ s,
 415 indicating that the fluctuations in the data are too significant to obtain meaningful averages. For $0.5 < w/d < 1$, the resulting fields are nearly parameter-independent, therefore $w = d$ is recommended for spatial averaging.

The study thus shows that the choice of both the spatial coarse-graining width and the time averaging interval are crucial to obtain meaningful field
 420 definitions in systems with highly localised, non-steady behaviour. No general rule for the choice of parameters is obtained, but the article outlines how to obtain the ideal set of parameters for the system studied – as a working example.

Once the CG parameters are selected, the macroscopic fields are used
 425 to study the flow patterns in the silo. To demarcate the three distinct flow regions, we look for a definition of the location and width of the shear bands. We observe that the tensorial shear rate $\dot{\gamma}$ and the inertial number are high in the left and right shear band (mainly simple shear) as well as in the core flow region (mainly pure shear). Thus, the horizontal gradient of vertical velocity,

430 $\partial_x v_z$, is used to define the (‘simple’) shear band, as it almost vanishes in the core flow region.

We compare three definitions for the shear band centre and width at a given height z : (a) the maximum and the 0.6-quantile of the shear rate, (b) the centroid and hygroscopic radius of the shear rate, and (c) the mean and
 435 standard deviation of a Gaussian fit to all shear rate values above the 0.6-quantile. Definition (c) is recommended, as for definition (a) both width and centre are dependent on the spatial resolution upon which the fit is made, and the width is strongly parameter-dependent in both definitions (a) and (b). Furthermore, the definition (c) of the width and centre are shown to be
 440 independent of w for $0.3 < w/d < 1$.

The stress analysis shows that the normal stresses are high in the stagnant region and nearly vanish in the flowing region. Furthermore, the normal stresses are highly anisotropic, with the downward stress much larger than the vertical stresses as would be expected in a silo condition [29, 30]. The
 445 stress is shown to transfer the weight of the flow to the walls, with the shear forces on the side walls carrying 21% and the base wall carrying 79% of the weight. Finally, the $\mu(I)$ rheology is addressed, which states that the ratio of shear and normal stresses in its objective form, μ , is a function of the inertial number, I , if the flow is in critical steady state. This is shown to be true for
 450 the shear zone, for $I > 0.1$, where the friction increases nearly linearly with the inertial number [15, 31].

The analysis of the flow rheology in this paper is by no means complete, as the focus of this paper was to investigate and find the optimal CG parameters. However, it proves that CG can provide meaningful results also

455 in non-homogeneous and non-steady situations. In a further publication on
this topic, we intend to analyse the stress tensor further to better understand
the many interesting phenomena that can be observed in these situations.
Examples are the strong stress anisotropy and the stick-slip behaviour near
the walls, the rheology and the dynamic behaviour of the shear band, and
460 the arch observed in the central flow region.

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