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THEME: [NMP.2013.1.4-1] Development of an integrated multi-scale modelling environment for nanomaterials and systems by design

Starting date of project: 1st of January, 2014

Duration: 48 months

WP N°	Del. N°	Title	Contributors	Version	Lead beneficiary	Nature	Dissemin. level	Delivery date from Annex I	Actual delivery date dd/mm/yyyy
5	5.1	Mesh-independent database of highly-resolved Euler-Euler simulation data	INPT	1.0	INPT, NTNU		PU	30/06/2015	30/10/2015

1 Executive summary

Modelling of dense gas-particle flows, using the Two Fluid Model (TFM) approach closed by the Kinetic Theory of Granular Flows (KTGF) is well established. However, recently it has been shown that for A-type particles, according to Geldart's classification, the numerical simulations fail to predict the behavior of the solid phase by the wrong prediction of the solid clusters. The use of subgrid models allows to take into account the effects of the unpredicted solid cluster on the "large-scale" behavior of the solid phase. For developing subgrid model, spatial filtering is applied on highly resolved numerical simulations using TFM.

Euler-Euler numerical simulations of binary mixture of solid particles in a Periodical Circulating Fluidized Bed have been carried out. The report gives all parameters used for performing the numerical simulations. An example of the statistics that can be extracted is also given. We recommend the reading of the references given at the end of the report.

2 Description of the numerical simulations

2.1 Configuration and specific developments

The configuration is the same than the one used for a previous study dedicated to monodisperse particles[1]. The size of the domain is described by Figure 1.

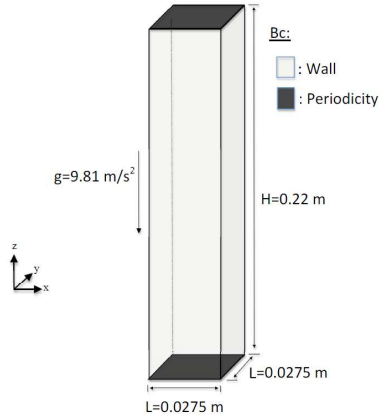

Figure 1: Geometry

Periodical boundary conditions are applied on the top and bottom of the geometry (in z-direction). All others boundaries are walls. For the gas, the wall-boundary conditions are No-slip and for the solid phase Free-slip boundary condition. The last represents the elastic bouncing of spherical particles on a smooth wall[2]. In such a configuration, a forcing method is applied to maintain a

[1] Ozel, A.; Fede, P. & Simonin, O. Development of filtered Euler-Euler two-phase model for circulating fluidised bed: High resolution simulation, formulation and a priori analyses International Journal of Multiphase Flow , 2013, 55, 43-63

[2] Fede, P.; Simonin, O.; Ansart, R.; Neau, H. & Ghouila, I. Effect of Wall Boundary Conditions and Mesh Refinement on Numerical Simulation of Pressurized Dense Fluidized Bed for Polymerization Reactor International Conference on Circulating Fluidized Beds and Fluidization Technology - CFB-10 May 1 - 5, Sunriver, Oregon, USA, 2011

constant whole momentum as we may found in the established zone of a real circulating fluidized bed. The forcing consists in an additional momentum source term:

$$F^{n+1} = \frac{(m_g + m_s)g}{V} + \frac{(1-\theta)}{V}\frac{M^* - M^n}{\Delta t}$$

where V is the volume of the domain, M^n the whole momentum (gas and particulate phases), and Δt the time step. M^* is the guessed value of the momentum and g the gravitational acceleration. In the following this value is set to zero. Using such a forcing, statically steady periodical circulating fluidized bed are obtained.

2.2 Numerical models

For performing the numerical simulations the following parameters have been used.

	Gas	***p*-Particle**	***q*-Particle**
Gas-particle momentum exchange	Gobin et al. (2001)	Gobin et al. (2001)	Gobin et al. (2001)
Particle-particle momentum exchange	-	Gourdel et al. (1998)	Gourdel et al. (1998)
Particle-particle agitation transfer and production terms	-	Gourdel et al. (1998)	Gourdel et al. (1998)
Turbulence modelling	Laminar	Particle agitation with additional terms for taking into account the polydispersion	Particle agitation with additional terms for taking into account the polydispersion
Collision modelling	-	Kinetic theory of granular media	Kinetic theory of granular media
Max compaction	-	0.64	0.64
Frictional effect	-	-	-

2.3 Material properties

The material properties of the gas are kept constant

- Density, $\rho_g = 1.18\ kg/m^3$
- Viscosity, $\nu_g = 1.8 \times 10^{-5} kg/m/s$

The density of the particles is also kept identical

- Density, $\rho_p = \rho_q = 1500\ kg/m^3$

The following Table gives the material properties of the particles for each investigated case.

Case	$d_p\ [\mu m]$	$d_q\ [\mu m]$	d_q/d_p	α_p	α_q	α_q/α_p	α_s
#1	75	150	2	3%	3%	1	6%
#2	75	150	2	1%	5%	5	6%
#3	75	150	2	2%	4%	2	6%

2.4 Meshes

For getting mesh-independent results severals meshes have been used.

Mesh	N_x	N_y	N_z	$N_{cell} = N_x \times N_y \times N_z$
M1	24	24	192	110 592
M2	32	32	256	262 144
M3	48	48	384	884 736
M4	64	64	512	2 097 152
M5	96	96	768	7 077 888

The cost of each simulation, namely for each mesh, is given in the following table. Obviously this time changes a little bit according to the material properties. Indeed, by changing the solid volume fraction the gas velocity of gas, or particles velocity, can increase and the time step decreases.

	Ncell	**Cpu Time/cycle**	**Physical time**	**Number of cores**
M1	262 144	0.906 s	8 s	20
M2	884 736	1.23 s	8 s	60
M3	2 097 152	2.28 s	~5.5 s	120
M4	7 077 888	5.57	~4 s	280

3 Results

3.1 Summary of the numerical simulations

Instantaneous fields are available for the following 15 numerical simulations.

	Mesh	$d_p\ [\mu m]$	$d_q\ [\mu m]$	d_q/d_p	α_p	α_q	α_q/α_p	α_s
1	M1	75	150	2	3%	3%	1	6%
2	M2							
3	M3							
4	M4							
5	M5							
6	M1	75	150	2	1%	5%	5	6%
7	M2							
8	M3							
9	M4							
10	M5							
11	M1	75	150	2	2%	4%	2	6%
12	M2							
13	M3							
14	M4							
15	M5							

3.2 Example of results

From each simulation spatial filtering is applied for measuring the contribution of each term coming from the filtered approach. It allows also to measure the correlation between each term in order to give some idea for developing a model.

The following results are coming from a simulation with the mesh M4. The material properties are those described above, and the numerical models as well. Only the solid volume fraction is different, $\alpha_p = 5\%$ and $\alpha_q = 1\%$.

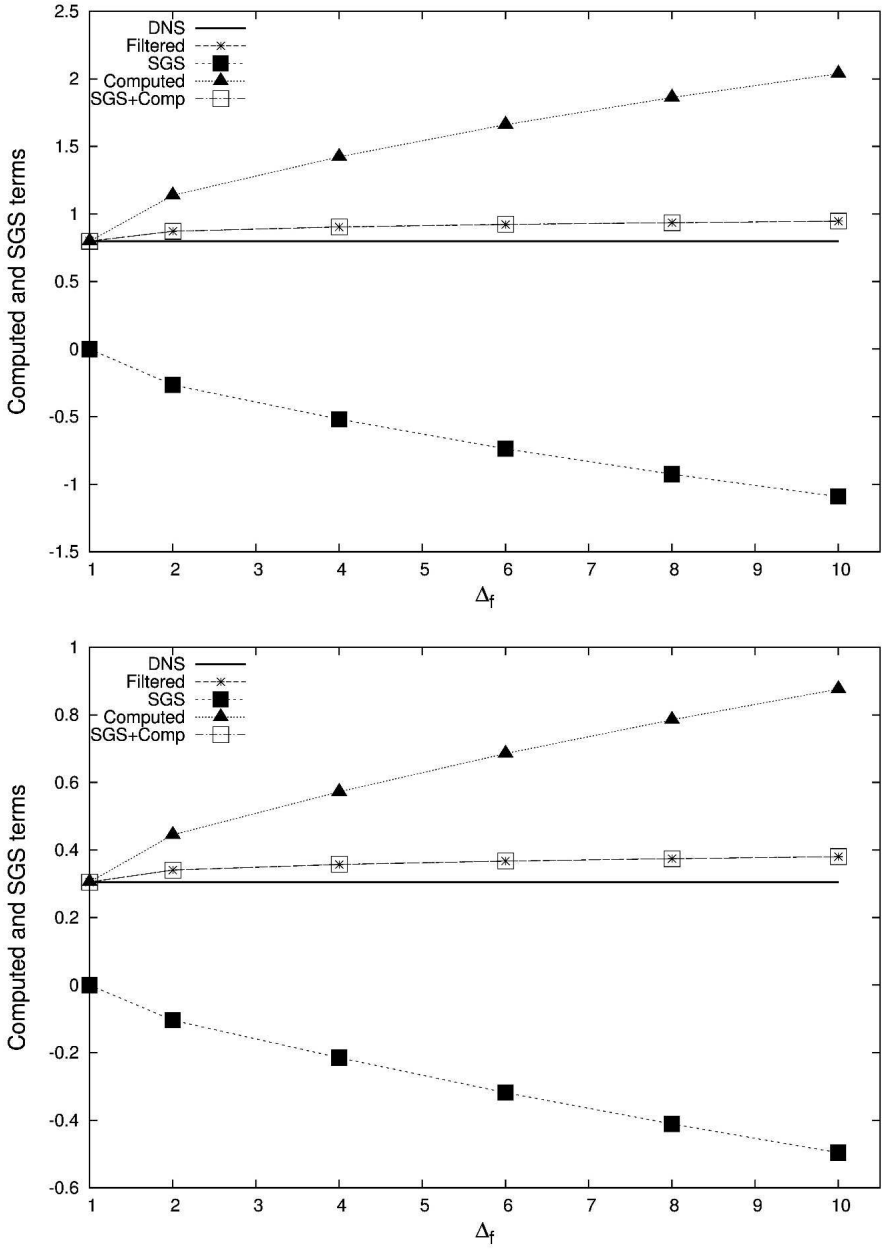

Figure 2. Drag contribution in momentum equation for p-particles (top) and q-particles (bottom)

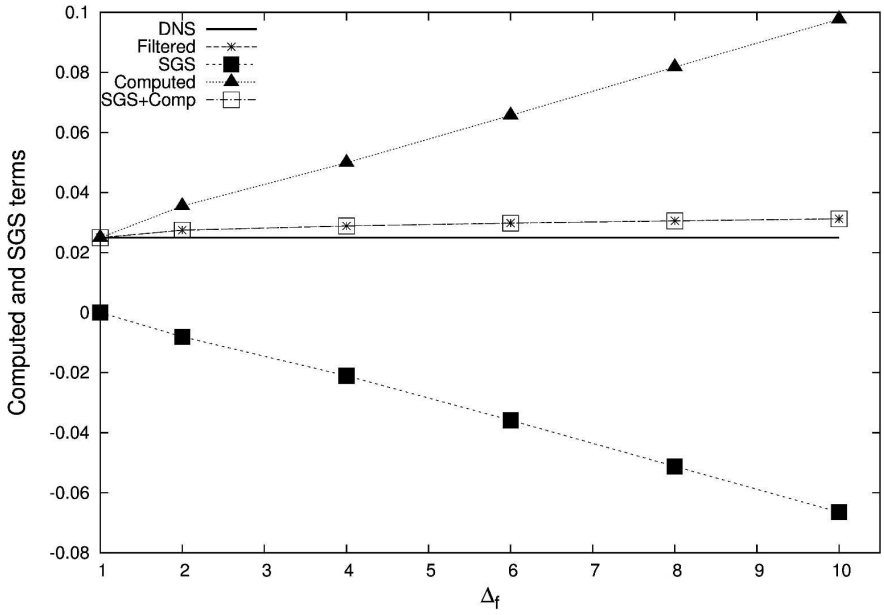

Figure 3. Inter-particle momentum contribution in the momentum equation

Figure 2 shows the drag contribution in the momentum equation for the two classes of particles. The filtered drag is defined by

$$Filtered = \frac{\alpha_p \rho_p}{\tau_p}\left(\widetilde{W_p} - W_g\right)$$

and the computed drag

$$Computed = \frac{\widetilde{\alpha_p}\rho_p}{\widetilde{\tau_p}}\left(\widetilde{W_p} - \widetilde{W_g}\right)$$

The subgrid drag contribution is then by definition given by

$$SGS = Filtered - Computed = \frac{\alpha_p \rho_p}{\tau_p}\left(\widetilde{W_p} - W_g\right) - \frac{\widetilde{\alpha_p}\rho_p}{\widetilde{\tau_p}}\left(\widetilde{W_p} - \widetilde{W_g}\right)$$

For the inter-particle collisions the momentum term writes:

$$Filtered = C n_p n_q g_r \widetilde{\left(W_p - W_q\right)} g_0 H_1(z)$$

where n_p is the mean particle number density, g_r the relative velocity between particles, and $H_1(z)$ a given function of the parameter

$$z = \frac{\left(\vec{U}_p - \vec{U}_p\right)^2}{\frac{8}{3}(q_p^2 + q_q^2)}$$

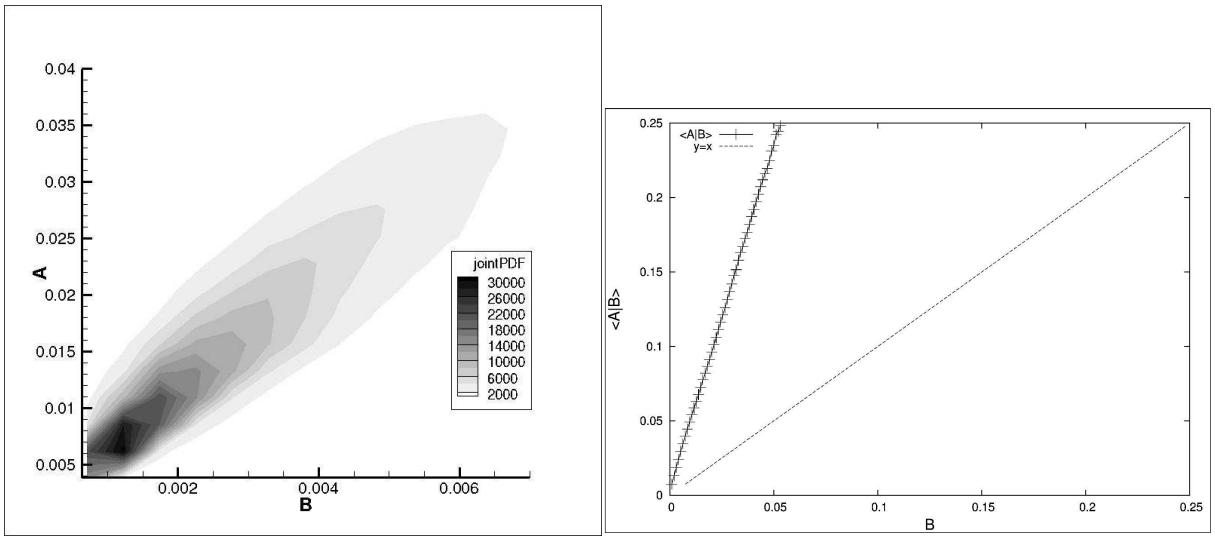

Figure 4. Correlation between the p-particle and the q-particle solid volume fraction. Left: Joint PDF and right conditioned averaging ($A = \alpha_p$ and $B = \alpha_q$).

Figure 3 shows the inter-particle momentum transfer term. The computed contribution writes

$$Computed = C\tilde{n}_p\tilde{n}_q\tilde{g}_r\left(\widetilde{W}_p - \widetilde{W}_q\right)\tilde{g}_0\widetilde{H_1}(z)$$

The subgrid scale contribution is also deduced from the de filtered and the Computed. Figure 4 shows the correlation between the two particle species. It shows that in domain the two particle species are present with the same proportion in the whole domain, here $\frac{\alpha_p}{\alpha_q} = 5$. For developing a subgrid model for the inter-particle collisions, we have to analyses the correlation between all ingredients of the inter-particle momentum transfer term. In the following we decompose step by step the momentum transfer term.

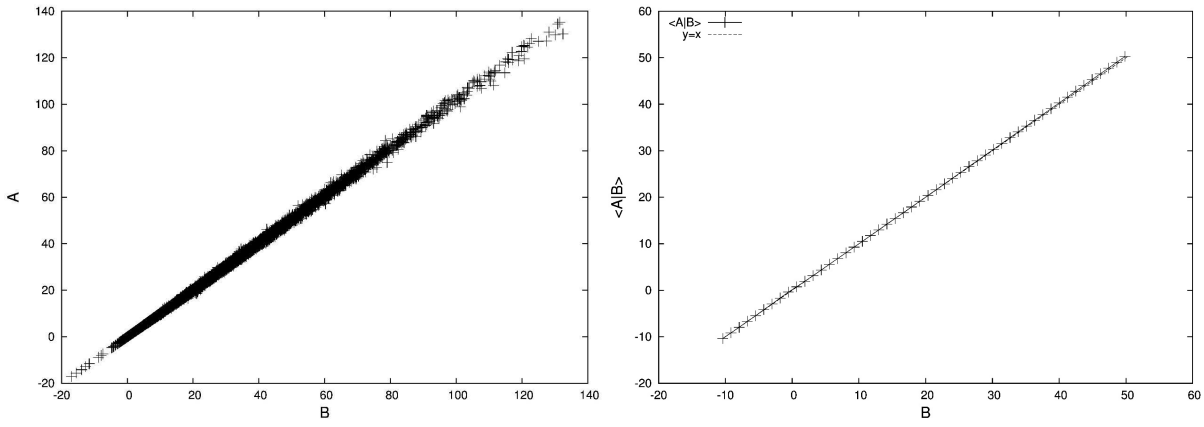

Figure 5. Effect of the function $H_1(z)$ on the filtered inter-particle momentum transfer. Here $A = Cn_pn_qg_r\widetilde{(W_p - W_q)}g_0H_1(z)$ $B = Cn_pn_qg_r\widetilde{(W_p - W_q)}g_0 \times \widetilde{H_1(z)}$

Figure 5 shows that the function $H_1(z)$ does not have an effect in the filtered inter-particle momentum transfer. The correlation between the two terms is almost 100%. This function does not have to be taken into account in the modelling.

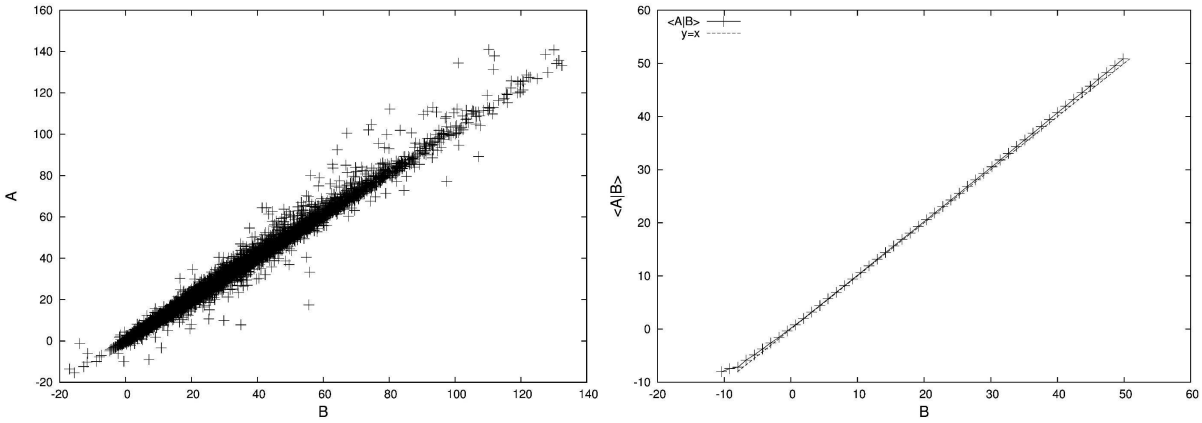

Figure 6. Effect of radial distribution function on the filtered inter-particle momentum transfer. . Here $A = Cn_p n_q g_r(\widetilde{W_p - W_q}) g_0 \times \widetilde{H_1(z)}$ and $B = Cn_p n_q g_r(\widetilde{W_p - W_q}) \times \widetilde{g_0} \times \widetilde{H_1(z)}$

The effect of the radial distribution function is shown by Figure 6. Here again, we can observe that the radial distribution function can be safely expressed with the computed variables without any effect on the terms representing the inter-particle momentum exchange.

The effect of the relative inter-particle velocity is shown by Figure 7. The figure shows that a correlation exists between the inter-particle momentum term and the relative velocity. In fact this is linked with the parameter z. Indeed, such a parameter allows to do the transition between a mean velocity dominated (large z) regime to an agitation-dominated regime (low value of z). In that case, the spatial averaged value of z is in a medium range meaning that the two regimes exist. More, we find two contributions in the mean inter-particle relative velocity g_r one for the mean relative velocity and one for the relative agitation.

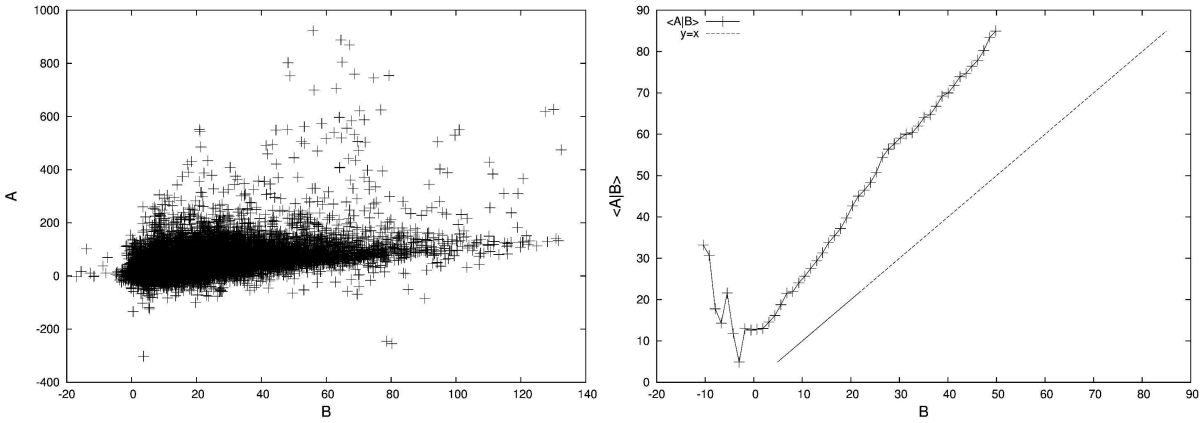

Figure 7. Effect of inter-particle relative velocity on the filtered inter-particle momentum transfer. Here $B = Cn_p n_q g_r(\widetilde{W_p - W_q}) \times \widetilde{g_0} \times \widetilde{H_1(z)}$ and $B = Cn_p n_q(\widetilde{W_p - W_q}) \times \widetilde{g_r} \times \widetilde{g_0} \times \widetilde{H_1(z)}$

4 Conclusions

The budget and correlation analysis show that the inter-particle momentum is affected by the mesh. The correlation analysis suggests that a subgrid inter-particle drift velocity exists and requires a modelling approach.

The data will be stored for being accessible by the community. A solution for sharing of data is being discussed due to the large space requirements (~1To). The format has been identified in order to be read by C3PO developed in the frame of NANOSIM.

5 Nomenclature

Latin symbols

- g_0: radial distribution function
- g_r: mean inter-particle relative velocity
- $H_1(z)$: transition function
- m_g: mass of gas in the computational domain
- m_s: mass of solid in the computational domain
- n_g: mean particle number density
- n_p: mean particle number density
- W_g: mean vertical gas velocity
- W_p: mean vertical particle velocity
- z: parameter quantifying the ratio between the mean inter-particle velocity and the mean relative agitation between the particles species

Greek symbols

- τ_p: particle response time
- ν_g: kinematic gas viscosity
- ρ_g: the particle density
- ρ_p: the p-particle density
- ρ_q: the q-particle density
- α_g: gas volume fraction
- α_p: solid volume fraction of p-particles
- α_q: solid volume fraction of q-particles
- $\alpha_s = \alpha_p + \alpha_q$: whole solid volume fraction
- α_{max}: maximum packing

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