NUMERICAL SIMULATION OF COLLISION DYNAMICS FOR FINITE SIZE PARTICLES IN TURBULENT SUSPENSION

S. Vincent, J.C. Brändle de Motta, E. Climent, J.-L. Estivalezes

ICMF 2016, Firenze, March 26th 2016











The particle laden flows

Numerical approach Collision model

Simulations

Particles dynamics Collisions Average flow around particles

Conclusion

Goals and outline

The main goal of this presentation is to:

Understand collisions for finite-size particles in a HIT.

The presentation follow those points:

- Context and motivations
- VoFLag method for finite size particles
- Lubrication phenomena and its model
- HIT characteristics
- Collisions in a HIT

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The particle laden flows

Particle laden flows are common:

In natural flows:

- Rivers
- Volcanos
- Clouds
- Microorganism
- In industrial applications:
 - Fluidized bed
 - Combustion Chamber

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Source: http://geography.unt.edu

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Source: Wikipedia

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Source: Wikipedia

Falkovich et al. - Nature - Vol. 4194 (2002).

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Source: Godfrey, NIWA

Durham et al. - Nature - 2148 (2013)

Denny et al. - Biological Bulletin - 203 (2002)

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- Combustion Chamber



Source: Linassier - Thèse Université de Toulouse (2012)

The particle laden flows

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In industrial applications:

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The particle laden flows

Many parameters drive those flows:

- Density Ratio
- Particle size
- Shape
- Flow
- Solid fraction
- **۱**...

Different numerical approaches exist:

- Microscopic
- Mesoscopic
- Macroscopic

Many parameters drive those flows:

- Microscopic (Fully Resolved Particles)
- Mesoscopic (Point-wise Particles)
- Macroscopic (Continuum phase)

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Many parameters drive those flows:

- Microscopic (Fully Resolved Particles)
- Mesoscopic (Point-wise Particles)
- Macroscopic (Continuum phase)



Microscopic method permits to understand surrounding fluid behaviour

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Method





Thetis code

- MAC staggered unstructured grid
- Finite volumes
- Fictitious Domain Approach

The solid behaviour is enforced by high viscosity.

Randrianarivelo et al. Int. J. Num. Meth. in Fluids (2005)

Vincent et al. - Comp. & Fluids (2007)

Vincent et al. - J. Comp. Phy. (2013)

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Collisions



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Collisions



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Collisions





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Collisions





A model is required.

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Collisions



$$\mathbf{F}_{\mathbf{I}}(\epsilon, \mathbf{u}_{\mathbf{n}}) = -6\pi\mu_{f}R\mathbf{u}_{n}\left[\lambda\left(\epsilon\right) - \lambda\left(\epsilon_{\mathsf{al}}\right)\right]$$

Brenner - Chem. Eng. Sci. - Vol. 16 (1961)

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Collisions



$$\mathbf{F}_{\mathbf{I}}(\epsilon, \mathbf{u}_{\mathbf{n}}) = -6\pi\mu_{f}R\mathbf{u}_{n}\left[\lambda\left(\epsilon\right) - \lambda\left(\epsilon_{al}\right)\right]$$

- µ_f dynamic viscosity
- R particle radius
- u_n normal velocity
- $\epsilon = \frac{d}{R}$ dimensionless distance
- λ Taylor series

Brenner - Chem. Eng. Sci. - Vol. 16 (1961)

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Collisions



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Collisions



$$\mathbf{F}_{s} = \underbrace{\frac{m_{e}\left(\pi^{2} + [lne_{d}]^{2}\right)}{[N_{c}\Delta t]^{2}}}_{\text{spring}} \mathbf{d} - \underbrace{\frac{2m_{e}\left[lne_{d}\right]}{[N_{c}\Delta t]}}_{\text{dashpot}} \mathbf{d}$$

Schäfer et al. - Jo. de Phys. - Vol 6 (1996)

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Collisions



$$\mathbf{F}_{s} = \underbrace{\frac{m_{e}\left(\pi^{2} + [\mathit{lne}_{d}]^{2}\right)}{[\mathit{N}_{c}\Delta t]^{2}}}_{\text{spring}} \mathbf{d} - \underbrace{\frac{2m_{e}\left[\mathit{lne}_{d}\right]}{[\mathit{N}_{c}\Delta t]}}_{\text{dashpot}} \dot{\mathbf{d}}$$

Schäfer et al. - Jo. de Phys. - Vol 6 (1996)

- *m_e* reduced mass
- *e_d* coefficient of restitution in vaccum
- *N_c* number of time step during collision
- Δt time step (fluid)

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Collisions



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Collisions



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Collisions



Collisions in turbulence

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Collisions





$$rac{e_l}{e_d} = exp\left(-rac{35}{St}
ight)$$

Legendre et al. - Phys. Fluids - Vol. 17 (2005)

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10²

St

 10^{3}

Collisions



Legendre et al. - Phys. Fluids - Vol. 17 (2005)

 St^*_C

10⁰

10¹

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Collisions





Legendre et al. - Phys. Fluids - Vol. 17 (2005)

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Introduction Numerical approach Simulations Conclusion Firenze, March 26th 2016

HIT: Initial condition



$$L_b = 2\pi$$

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Introduction Numerical approach Simulations Conclusion Firenze, March 26th 2016

HIT: Initial condition



$$L_b = 2\pi$$
$$\frac{L_b}{\Lambda} = 2\pi$$
HIT: Initial condition



$$L_b = 2\pi$$
$$\frac{L_b}{\Lambda} = 2\pi$$
$$\frac{\Lambda}{\lambda} = 4.3$$

HIT: Initial condition



$$L_b = 2\pi$$

 $\frac{L_b}{\Lambda} = 2\pi$
 $\frac{\Lambda}{\lambda} = 4.3$
 $\frac{\eta}{\lambda} = 17$

HIT: Initial condition



$$L_b = 2\pi$$
$$\frac{L_b}{\Lambda} = 2\pi$$
$$\frac{\Lambda}{\lambda} = 4.3$$
$$\frac{\eta}{\lambda} = 17$$
$$\frac{R_p}{\eta} = 11$$

Collisions in turbulence

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 $\frac{L_b}{\Lambda}$

 $\frac{\Lambda}{\lambda}$

HIT: Initial condition



$$Re_{\lambda} = 73$$

$$Re_{\Lambda} = 315$$

$$L_{b} = 2\pi$$

$$\frac{L_{b}}{\Lambda} = 2\pi$$

$$\frac{\rho_{p}}{\rho_{f}} = \{1, 2, 4\}$$

$$\frac{\Lambda}{\lambda} = 4.3$$

$$St_{k} = 26\frac{\rho_{p}}{\rho_{f}}$$

$$St_{E} = 1.5\frac{\rho_{p}}{\rho_{f}}$$

$$\frac{\eta}{\lambda} = 17$$

$$R_{p}}{\eta} = 11$$

$$M_{p} = 512$$

$$\phi_{v} = 3\%$$

$$\frac{\eta_{k}}{\Delta x} = 0.56$$
Nodes = 256³

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HIT: Initial condition



 $Re_{\lambda} = 73$ $Re_{\Lambda} = 315$ $L_b = 2\pi$ $\frac{L_b}{\Lambda} = 2\pi$ $\frac{\rho_p}{\rho_f} = \{1, 2, 4\}$ $rac{\Lambda}{\lambda} = 4.3$ $St_k = 26rac{
ho_p}{
ho_f}$ $St_E = 1.5rac{
ho_p}{
ho_f}$ $\frac{\eta}{\lambda} = 17$ $\frac{R_p}{\eta} = 11 \quad \begin{array}{c} N_p = 512\\ \phi_v = 3\% \end{array}$ $\frac{\eta_k}{\Delta x} = 0.56$

 $\frac{\eta_{\kappa}}{\Delta x} = 0.56$ Nodes = 256³

The particles are on the inertial range.

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HIT: Initial condition



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HIT: Initial condition



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HIT: Initial condition



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HIT: Initial condition



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HIT: Initial condition



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Visualization of one simulation

512 particles

256³ grid nodes 512 processors

 \sim 10h / T_E

(Movie)

In this section only solid collision model is activated (no lubrication).

Collision time



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Collision time



$$\frac{1}{\tau_c} = n_p \pi d_p^2 < |\mathbf{w}| >$$

Collision time



$$egin{aligned} rac{1}{ au_c} &= n_p \pi d_p^2 < |\mathbf{w}| > \ &< |\mathbf{w}| > = < |\mathbf{V}_p^a - \mathbf{V}_p^b| > \end{aligned}$$

Collision time



$$\begin{split} & \frac{1}{\tau_c} = n_p \pi d_p^2 < |\mathbf{w}| > \\ & \frac{1}{\tau_c^{\text{th}}} = n_p \pi d_p^2 \sqrt{\frac{16}{\pi} \frac{2}{3} q_p^2} \end{split}$$

Collision time



$$\frac{1}{\tau_c} = n_p \pi d_p^2 < |\mathbf{w}| >$$
$$\frac{1}{\tau_c^{\text{th}}} = n_p \pi d_p^2 \sqrt{\frac{16}{\pi} \frac{2}{3}} q_p^2$$

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Collision time



Saffman and Turner - J. Fluid. Mech. - Vol. 1 (1956)

Collision time



Collision time



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Contact angle



The velocity between particles at collision are correlated.

Collision velocity

Effect of the lubrication on intercollision time

Visualization of secondary collisions

 $\rho=1$ with lubrication model

Encounter
 Solid collision (Movie)

Effect of lubrication in acceleration p.d.f

Collisions increase the p.d.f. for large accelerations.

Comparison for different density ratio



Effect of lubrication in acceleration p.d.f

Collisions increase the p.d.f. for large accelerations.

Suppress accelerations during collision



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Effect of lubrication in acceleration p.d.f

Collisions increase the p.d.f. for large accelerations.

Acceleration r.m.s. is related to density. $A_0 = a_{r.m.s.}^2/\epsilon^{3/2}\nu^{1/2}$

Qureshi et al. - European Phy. Jo. B - 2008



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Effect of lubrication in acceleration p.d.f

Collisions increase the p.d.f. for large accelerations.

Suppress accelerations during collision



Effect of lubrication in acceleration p.d.f

Collisions increase the p.d.f. for large accelerations.

Exponential Count coll 10⁻¹ No count €. 10⁻² 10⁻² 10⁻³ 10^{-4} -15 -10 -5 0 5 10 15 a / a_{rms}

Comparison for $\rho=1$

Effect of lubrication in acceleration p.d.f

Collisions increase the p.d.f. for large accelerations.

Same but for lubricated case



The lubrication do not modify the p.d.f. for larger accelerations

Conclusions and future work

This work highlight some important effects:

- > The lubrication model is representative for collisions in viscous fluids
- The lubrication creates the secondary collisions
- This secondary collisions have an effect on collision time
- The collisions modify the acceleration p.d.f.

These effects have to be considered when the collision frequency is treated. New models have to be put in place.

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Appendix

Appendix: Method VoFLag method Simulation Collision Particle Stats Average flow calculation Validations Poiseuille Rotation Sedimentaition Job time







- MAC stagered grid
- Finite volumes
- Fictitious Domain Approach



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$\mathbf{X}_{i}^{n}, \mathcal{R}_{i} \longrightarrow \mathbf{Find nodes on particles} \longrightarrow \mathbf{Treat particles} on borders} \longrightarrow \mathbf{Update density} p^{n}, \mu^{n}$



The solid behaviour is enforced by high viscosity.

Randrianarivelo et al. Int. J. Num. Meth. in Fluids - Vol. 47

(2005)

Vincent et al. - Comp. & Fluids - Vol. 36 (2007)

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$$\widetilde{\mathbf{X}_{i}^{n+\frac{1}{2}} = \mathbf{X}_{i}^{n} + \frac{\Delta t}{2}\mathbf{V}_{i}^{n}t}$$
$$\widetilde{\mathbf{V}_{i}^{n+\frac{1}{2}} = \frac{3}{2}\mathbf{V}_{i}^{n} - \mathbf{V}_{i}^{n-1}}$$

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A collision model gives the force applied on each particle. The model developed is explained in later.

Brändle et al. - Phys. Fluids - (2013)

Breugem - ASME Summer Meeting - Montreal (2010)

Method





The force is distributed on the solid volume and becomes a source term for N.-S. solution.





An augmented Lagrangian method is implemented. With BiCG Stab solver.





The new velocity field is calculated. The solid behaviour is respected by this field.

Vincent et al. - Comp. & Fluids - Vol. 36. (2007)



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Method





The particle velocity is calculated by interpolating the velocity





Method





$$\left(\mathbf{X}_{i}^{n+1}=\mathbf{X}_{i}^{n}+\Delta t\left(\frac{\mathbf{V}_{i}^{n+1}+\mathbf{V}_{i}^{n}}{2}\right)\right)$$

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Validations





Dennis et al. - JFM - Vol 101 (1980)



Validations



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Validations



Constraints



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Constraints



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Constraints



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Constraints



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Constraints



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Constraints



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Constraints



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HIT: Forcing

The turbulence forcing is done in physical space by maintaining the total energy

$$u_n = \sqrt{\frac{E_0}{E_n}}$$

(the density of particles is not taken into account)

Rosales et. al - Phys. Fluids - Vol. 17 (2005)

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HIT: Turbulence modulation



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HIT: Turbulence modulation



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HIT: Turbulence modulation



 $\Rightarrow~$ We need to analyze the Lagrangian spectrum

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HIT: Lagrangian spectrum

Fluid particles

Collisions in turbulence

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HIT: Lagrangian spectrum



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HIT: Lagrangian spectrum



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Intercollision time



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ρ	q_p^2	$\frac{q_p^2}{q_f^2}$	T_L	$\frac{T_L}{T_L^f}$	D	$\frac{D}{D_f}$
-	$(m^2 s^{-2})$	-	<i>(s)</i>	-	$(m^2 s^{-1})$	-
1	1.27	0.85	1.22	1.31	3.10	1.13
2	1.17	0.79	1.35	1.45	3.16	1.15
4	1.10	0.74	1.53	1.65	3.37	1.23

ρ	q_p^2	$\frac{q_p^2}{q_f^2}$	T_L	$\frac{T_L}{T_L^f}$	D	$\frac{D}{D_f}$
-	$(m^2 s^{-2})$	-	<i>(s)</i>	-	$(m^2 s^{-1})$	-
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2	1.17	0.79	1.35	1.45	3.16	1.15
4	1.10	0.74	1.53	1.65	3.37	1.23

The q_p^2 agitation decreases with ρ .

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ρ	q_p^2	$\frac{q_p^2}{q_f^2}$	T_L	$\frac{T_L}{T_L^f}$	D	$\frac{D}{D_f}$
-	$(m^2 s^{-2})$	-	<i>(s)</i>	-	$(m^2 s^{-1})$	-
1	1.27	0.85	1.22	1.31	3.10	1.13
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4	1.10	0.74	1.53	1.65	3.37	1.23

The velocity autocorrelation time T_L increases with ρ .

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ρ	q_p^2	$\frac{q_p^2}{q_f^2}$	T_L	$\frac{T_L}{T_L^f}$	D	$\frac{D}{D_f}$
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1	1.27	0.85	1.22	1.31	3.10	1.13
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-	$(m^2 s^{-2})$	-	<i>(s)</i>	-	$(m^2 s^{-1})$	-
1	1.27	0.85	1.22	1.31	3.10	1.13
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4	1.10	0.74	1.53	1.65	3.37	1.23

 q_p^2 and T_L balance and give similar diffusion coefficient.

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Particles diffusion



$$\frac{D}{D_f} = \frac{2q_p^2 T_L}{2q_f^2 T_L^f} = \{1.13, 1.15, 1.23\}$$
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Average flow calculation



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Average flow calculation



Collisions in turbulence

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Average flow calculation



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Average flow calculation



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Collisions in turbulence

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Average flow calculation



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Validations

lci je vais mettre les slides que j'avais fait sur les validations afin de répondre aux questions

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Validations: Poiseuille



Segré and Silberberg - Nature - Vol. 189 (1961)

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Validations: Poiseuille



Equilibrium

Segré and Silberberg - Nature - Vol. 189 (1961)

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Validations: Poiseuille

A : Inamuro et al. - IJMF - Vol 26 - 2000

B : Pan et al. - JCP - Vol 181 - 2002

	Author	Case1	Case2	Case3	Case4	Case5	Case6
$Re = \frac{L\overline{u_f}}{\mu}$		12.78	27.72	43.40	55.55	69.13	96.74
Ŧ	A	0.2745	0.2733	0.2728	0.2723	0.2716	0.2706
	В	0.2732	0.2725	0.2723	0.2720	0.2719	0.2722
	VofLag	0.2643	0.2636	0.2637	0.2643	0.2650	0.2752
	Error	3.8%	3.6%	3.4%	3.0%	2.5%	2.0 %
Ū	A	0.04137	0.04131	0.04091	0.04118	0.04110	0.04101
	В	0.04155	0.04159	0.04122	0.04166	0.04148	0.04144
	VofLag	0.04599	0.04605	0.04570	0.04628	0.04623	0.04682
	Error	10.6%	10.9%	11.1%	11.7%	11.7%	13.2%
	A	-0.054675	-0.054694	-0.053772	-0.053765	-0.053101	-0.051607
ω	В	-0.05345	-0.05343	-0.05264	-0.05264	-0.05206	-0.05052
	VofLag	-0.05500	-0.05331	-0.05082	-0.04966	-0.04761	-0.05276
	Error	0.6%	2.6%	5.6%	7.9%	10.9%	2.2%

With 6 nodes per diameter we obtain a low relative error

Method Simulation Collision Particle Stats Average flow Validations Job time Firenze, March 26th 2016

Validations : Dennis 1980



Collisions in turbulence

Method Simulation Collision Particle Stats Average flow Validations Job time Firenze, March 26th 2016

Validations : Dennis 1980





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Method Simulation Collision Particle Stats Average flow Validations Job time Firenze, March 26th 2016

Validations : Dennis 1980



Collisions in turbulence

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Validations : Dennis 1980

Dimensionless torque $M = \frac{2T}{\rho_f R^5 \omega^2}$ vs Reynolds number $Re_\omega = \frac{R^2 \omega \rho}{\mu_f}$



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Validations: Ten Cate 2002



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Firenze, March 26th 2016

Validations: Ten Cate 2002



37/19

HIT : Jobs time

With 512 procs

	$T_{\rm sim}/T_E$	Percentage
Navier-Stokes Resolution	26828 <i>s</i>	75%
Postraitement (Out + Spectra)	3977 <i>s</i>	11%
Fluid Particles	2121 <i>s</i>	6%
Advection	2105 <i>s</i>	6%
Collisions	39 <i>s</i>	< 1%
Others	714 <i>s</i>	2%
Total	35784 $s\sim 10~{ m h}$	