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# Modulation of homogeneous and isotropic turbulence by sub-Kolmogorov particles: impact of particle field heterogeneity

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## Abstract

The modulation of turbulence by sub-Kolmogorov particles has been thoroughly characterized in the literature, showing either enhancement or reduction of kinetic energy at small or large scale depending on the Stokes number and the mass loading. However, the impact of a third parameter, the number density of particles, has not been independently investigated. In the present work, we perform direct numerical simulations of decaying Homogeneous Isotropic Turbulence loaded with monodisperse sub-Kolmogorov particles, varying independently the Stokes number, the mass loading and the number density of particles. Like previous investigators, crossover and modulations of the fluid energy spectra are observed consistently with the change in Stokes number and mass loading. Additionally, DNS results show a clear impact of the particle number density, promoting the energy at small scales while reducing the energy at large scales. For high particle number density, the turbulence statistics and spectra become insensitive to the increase of this parameter, presenting a two-way asymptotic behavior. Our investigation identifies the energy transfer mechanisms, and highlights the differences between the influence of a highly concentrated disperse phase (high particle number density, limit behavior) and that of heterogeneous concentration fields

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(low particle number density). In particular, a measure of this heterogeneity is proposed and discussed which allows to identify specific regimes in the evolution of turbulence statistics and spectra.

*Keywords:* Particle dynamics, homogeneous isotropic turbulence, two-way coupling, heterogeneity.

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### **Highlights**

- Original and exhaustive study of sub-Kolmogorov particle - turbulence two-way interactions for decreasing HIT.
- Beyond the usual influence of Stokes and mass loading, study of impact of the particle number density.
- Influence of particle phase heterogeneity on spectral distribution of energy coupling is investigated and characterized.
- Design of a heterogeneity measure and criterion for convergence of turbulence statistics.

### **Introduction**

Turbulent flows laden with particles or droplets are common in many engineering and environmental applications, such as atmospheric dispersal of pollutants, liquid sprays in engines, sediments in rivers, droplets in clouds etc. The turbulence can completely govern the particles' behavior, and in the case of sufficiently dense flows, the presence of particles can also influence the turbulence (Squires and Eaton, 1990; Boivin et al., 1998).

In the literature, the interactions between a turbulent carrier phase and a particulate phase in the point-particle limit have been extensively studied. In the one-way coupled context, for which the particles do not affect the carrier phase, the importance of Stokes number based on Kolmogorov or Lagrangian integral time scales have

been demonstrated: the former characterizes the occurrence of preferential concentration (Eaton and Fessler, 1994) while the latter is representative of the transition to particle-trajectory-crossing dominated flows (Février et al., 2005).

In the case of two-way coupling, turbulence modulation by particles has been also investigated in Homogeneous Isotropic Turbulence (HIT), focusing on the effect of the Stokes number and mass loading. On the one hand, studies on stationary HIT of Squires and Eaton (1990); Boivin et al. (1998); Mallouppas et al. (2017) showed that the turbulent kinetic energy of the carrier phase is reduced by particles. They concluded that inertial particles inject energy in the turbulent motion at high wavenumbers with a corresponding increase in the dissipation, which was also described by Squires and Eaton (1994) with respect to mass loading.

On the other hand, Elghobashi et al. (1994); Druzhinin and Elghobashi (1999); Druzhinin (2001); Ferrante and Elghobashi (2003); Abdelsamie and Lee (2012) worked with a decaying HIT and found that particles with low Stokes number can enhance the fluid energy. Indeed, studies on the fluid-particle interaction spectrum reveal a negative contribution at low wave numbers where intensity is reduced when Stokes number increases, whereas the energy rate at large wavelengths remains positive. More generally, Ferrante and Elghobashi (2003) classified particles according to their Stokes number and described the evolution of turbulent energy and dissipation of the flow, and Sundaram and Collins (1999) showed that the shift in energy to high wavenumbers in the fluid phase increases the viscous dissipation rate. The focus of all these studies was the influence of the Stokes number and mass loading: the former parameter globally determines the dynamics of particles in a given fluid and the latter plays a role in the inverse-coupling force that the particles exert on the fluid. Table 1 summarizes some of the previous works, and the parameters studied.

A dimensional analysis leads to the identification of a third controlling parameter, the particle number density. In fact, this parameter plays a key-role: for high number density, the proximity of particles can lead to a continuous phase behavior, while for low number density, distant particles can produce strong local effects on the surrounding fluid and the exact location of the particles may have a great impact on the dynamics of the flow, depending on the realization. In the literature, this parameter has

Reference	Forcing	$M_r/M_c$	Fixed	Changed
Squires and Eaton (1990)	YES	100	$\tau_p, n_0$	$\phi, \alpha, \rho_p, d_p$
Elghobashi et al. (1994)	NO	100	$\alpha, \tau_p$	$d_p, \phi, n_0, \rho_p$
			$\alpha, d_p, n_0$	$\tau_p, \rho_p, \phi$
			$\tau_p, \rho_p, d_p$	$\alpha, \phi, n_0$
Squires and Eaton (1994)	YES	1	$\tau_p, n_0$	$\phi, \alpha, \rho_p, d_p$
Boivin et al. (1998)	YES	$> 1$	$\alpha, \phi, \rho_p$	$\tau_p, d_p, n_0$
			$\tau_p, n_0$	$\phi, \rho_p, \alpha, d_p$
Druzhinin and Elghobashi (1999)	NO	1	$\tau_p, \rho_p, d_p$	$\phi, \alpha, n_0$
Sundaram and Collins (1999)	NO	1	$\alpha, \phi, \rho_p$	$\tau_p, d_p, n_0$
			$\tau_p, d_p, \rho_p$	$\alpha, \phi, n_0$
Druzhinin (2001)	NO	1	$\alpha, \phi, \rho_p$	$\tau_p, d_p, n_0$
Ferrante and Elghobashi (2003)	NO	47	$\alpha, \phi, \rho_p$	$\tau_p, d_p, n_0$
Abdelsamie and Lee (2012)	YES vs NO	95	$\alpha, \phi, \rho_p$	$\tau_p, d_p, n_0$
Mallouppas et al. (2017)	YES	1	$\alpha, d_p, n_0$	$\tau_p, \rho_p, \phi$
			$\tau_p, \rho_p, d_p$	$\phi, \alpha, n_0$

**Table 1:** Previous studies of the modulation of turbulence by disperse phase. Forcing scheme for stationary HIT and ratio of real particles per computational particle are precised for each study. Choice of fixed parameters and studied parameters are displayed in the two last columns. In the table,  $\tau_p$  is the particle relaxation time,  $\alpha$  is the volume fraction,  $n_0$  is the particle number density,  $\phi$  is the mass fraction,  $\rho_p$  is the particle density and  $d_p$  is the diameter of particles.

been first studied in the objective of reaching statistical convergence for one-way coupled simulations (Vié et al., 2016). Strutt et al. (2011) observed the lack of consensus regarding the number of particles that must be considered in simulations. A common definition for statistical convergence is the point at which the particle dispersion statistics do not change significantly (i.e. become independent on the number of particles). On the other hand, Sundaram and Collins (1999) studied a regime with very low particle number density, for which each particle acts independently and observed that their collective effect on the fluid scales linearly with the total number of particles.

In the present work, we investigate the effect of the particle number density along with the mass loading and the Stokes number. We propose a characterization and a measure for the heterogeneity of the particulate phase. We identify two regimes in two-way coupled flows, according to the level of heterogeneity of the disperse phase: an asymptotic behavior for highly-concentrated particle phase (high particle number density), and a strong response of turbulence at small scales for the heterogeneous particle phase. We provide some characterization of turbulence statistics and energy spectra for those specific regimes and explain the transition between them for intermediary particle number densities.

In section 1, we first present the assumptions and governing equations of our study, as well as the numerical methods. Then, the target HIT configuration and the parameter set are presented in section 2, with an emphasis on the other parametric studies in the literature. A definition of heterogeneity is detailed in section 3 along with the way to measure it unequivocally when preferential concentration occurs. Results of the extensive study are presented in section 4, in the following order: turbulence modulation by particles is measured through the analysis of global energy transfers (section 4.1). Then, deeper insight is given by an analysis in the spectral domain (section 4.2), permitting to identify specific regimes with respect to the number density of the particulate phase. These regimes are further analyzed in section 4.3, in particular with regard to coupling mechanisms.

## 1. Modeling and numerical frameworks

### 1.1. Fluid and particles equations

We consider monodisperse solid spherical particles of fixed size. Particles diameter is smaller than the Kolmogorov length scale ( $d_p \ll \eta$ ), thus particle-resolved DNS is not necessary (Fröhlich et al., 2018), and a point-particle approximation is adopted. The density ratio between the particles and the fluid is large ( $\rho_p \gg \rho_f$ ) and the Reynolds number of the particle is smaller than one ( $Re_p \leq 1$ ). The volume fraction  $\alpha$  is small enough to consider particle-particle collisions as negligible (dilute regime:  $\alpha < 10^{-3}$ ). Therefore, many of the forces in the original Basset-Boussinesq-Oseen equation are assumed negligible compared to the drag force. Furthermore, if the drag force obeys Stokes' law, the equation of motion is linear in the velocity difference between fluid and particle. Then the motion equations of particles are written as

$$\begin{cases} \frac{d\mathbf{x}_p(t)}{dt} = \mathbf{v}_p(t) \\ \frac{d\mathbf{v}_p(t)}{dt} = \frac{\mathbf{u}_{f@p}(t) - \mathbf{v}_p(t)}{\tau_p} \end{cases} \quad (1)$$

where  $\mathbf{x}_p(t)$  and  $\mathbf{v}_p(t)$  stand for particle position and velocity at time  $t$ , and  $\mathbf{u}_{f@p}(t) = \mathbf{u}_f(t, \mathbf{x}_p(t))$  is the fluid velocity evaluated at the particle position. The particle relaxation time  $\tau_p$  is defined as  $\tau_p = \frac{\rho_p d_p^2}{18\mu_f}$  where  $\mu_f$  is the dynamic viscosity of the fluid. The effects of particles on the carrier phase are expressed through an additional force in the momentum equation of the fluid. For an incompressible fluid, the equations of motion for the carrier fluid are:

$$\begin{cases} \frac{\partial u_{f,i}}{\partial x_i} = 0 \\ \frac{\partial u_{f,i}}{\partial t} + \frac{\partial u_{f,i} u_{f,j}}{\partial x_j} = \frac{-1}{\rho_f} \frac{\partial P}{\partial x_i} + \frac{\mu_f}{\rho_f} \frac{\partial^2 u_{f,i}}{\partial x_j \partial x_j} + \frac{1}{\rho_f} f_i \end{cases} \quad (2)$$

where  $\mathbf{f}$  is the force exerted by particles on the fluid.

### 1.2. Coupling equations

A projection kernel  $\Delta$  is introduced to give a local average of the feedback force. This function is positive, monotonically decreasing and normalized such that its integral

over the entire physical space is unity. The source term  $\mathbf{f}$  in Eq.2 is then written as:

$$\mathbf{f}(\mathbf{x}, t) = \sum_p \mathbf{F}^{(p)} \Delta(\mathbf{x} - \mathbf{x}_p(t)) \quad (3)$$

where  $\mathbf{F}^{(p)} = m_p \frac{\mathbf{v}_p(t) - \mathbf{u}_{f@p}(t)}{\tau_p}$  is the resultant force exerted by a particle  $p$  of mass  $m_p$  on the fluid.

Other Eulerian spatial fields can therefore be defined as:

$$n(\mathbf{x}, t) = \sum_p \Delta(\mathbf{x} - \mathbf{x}_p(t)) \quad (4)$$

$$n(\mathbf{x}, t) \tilde{\mathbf{v}}_p(\mathbf{x}, t) = \sum_p \mathbf{v}_p \Delta(\mathbf{x} - \mathbf{x}_p(t)) \quad (5)$$

$$n(\mathbf{x}, t) \tilde{\mathbf{u}}_{f@p}(\mathbf{x}, t) = \sum_p \mathbf{u}_{f@p} \Delta(\mathbf{x} - \mathbf{x}_p(t)) \quad (6)$$

Spatial averages can then be derived and the notation used is  $\langle f(\mathbf{x}, t) \rangle = \frac{1}{|\mathcal{V}_f|} \int_{\mathcal{V}_f} f(\mathbf{x}, t) d\mathbf{x}$ , where  $\mathcal{V}_f$  indicates that the integral is taken over the whole domain of fluid  $|\mathcal{V}_f| = L^3$ . For monodisperse spherical particles,  $m_p = \rho_p \pi d_p^3 / 6$  and global volume fraction is defined as  $\alpha = n_0 \pi d_p^3 / 6$ , where  $n_0$  is the mean particle number density  $\langle n(\mathbf{x}, t) \rangle = n_0$ . The mass loading of the disperse phase is therefore defined as  $\phi = \alpha \rho_p / \rho_f$ . To highlight the effect of these parameters, the coupling term is expressed as:

$$\frac{1}{\rho_f} \mathbf{f}(\mathbf{x}, t) = \phi \frac{n(\mathbf{x}, t)}{n_0} \frac{\tilde{\mathbf{v}}_p(\mathbf{x}, t) - \tilde{\mathbf{u}}_{f@p}(\mathbf{x}, t)}{\tau_p} \quad (7)$$

The mass fraction term is thus a factor in the expression, the fraction  $\frac{n(\mathbf{x}, t)}{n_0}$  contains information about the spatial distribution of particles and the last term is related to the Stokes number.

### 1.3. Numerical methods

We performed direct numerical simulation to solve the unsteady three-dimensional Navier-Stokes and continuity equations with the Asphodele code using a low Mach formulation of the Navier-Stokes equations and a Lagrangian formulation for the particles. This code was developed by J. Réveillon and co-workers at CORIA laboratory (Reveillon and Demoulin, 2007). The time resolution is provided by a third order



explicit Runge Kutta scheme and spatial evolution is done with a high order finite difference scheme.

One of the key aspects of in Euler-Lagrange simulation is the coupling between the particle equations and the carrier phase. Two elements are required: an interpolation scheme to evaluate the gas phase properties at the particle locations, and a projection scheme to compute the feedback of particles to the gas phase or to compute particle Eulerian fields.

For the interpolation step, we use a third-order algorithm to compute the gaseous quantities at droplet location. Strutt et al. (2011) discussed the accuracy of interpolation schemes such as the fourth-order cubic spline, the fifth-order Lagrange or the third-order Hermite polynomials interpolation.

The choice of the projection kernel depends on the developed physics or the desired precision. The PSI-Cell method of Crowe et al. (1977) was originally implemented in Asphodele code. The Lagrangian contributions are instantaneously allocated to neighboring gas nodes, weighted by the distance to the nodes. This procedure is sometimes controversial because it leads to significant error that depends on the ratio of particle diameter to the grid spacing. This approach requires for the mesh size to be much larger than the particle diameter. More physical mollification kernels can be used to transfer particle data on the Eulerian mesh, such as described by Capecelatro and Desjardins (2013). Diffusion operation might also be necessary to deal with finer grids. Maxey et al. (1997) proposed a "narrow envelope function" in the form  $\Delta(\mathbf{x}) = (2\pi\sigma^2)^{-3/2} \exp(-\mathbf{x}^2/2\sigma^2)$ , which was used by other works (Capecelatro and Desjardins, 2013; Zamansky et al., 2014). The length scale  $\sigma$  is a parameter that can be adjusted to reflect the finite size of the particle. A gaussian envelope for the source term was also implemented in the code and a comparison of the influence of the projection kernels is provided in Appendix A: the effect of the coupling kernel is limited to the smallest scales and does not impact the qualitative results that are reported in this work.

## 2. Target configuration and parameter sets

### 2.1. Homogeneous Isotropic Turbulence

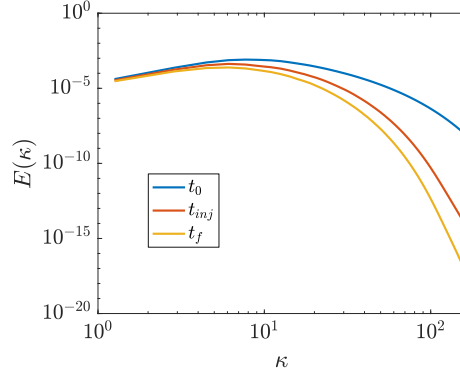
Among the works mentioned in the introduction, we can distinguish studies with forced stationary turbulence, for which statistics are therefore easier to carry out, from naturally decreasing turbulences, as reported in Table 1. A comparison of these turbulences is proposed by Abdelsamie and Lee (2012), who noted a number of difficulties in the attempt to study the impact of particles on the energy spectrum when it is artificially forced. Many differences are observed, including significant changes in the influence of small particles that do not allow energy to be reintroduced to the fluid in forced turbulence. And although Mallouppas et al. (2013) introduced a new forcing model, the same biases observed for small particles are found in their results. We have therefore chosen a configuration of decaying turbulence, for which we normalize the observed quantities by the total kinetic energy at each instant and thus retrieve more stationary trends in the evolution of components of the energy decay rate.

The proposed test case is a decaying homogeneous isotropic turbulence loaded with particles. The domain is a cubic periodic box of size  $L = 5$  meshed with  $N_g^3 = 256^3$  cubic cells. The initial condition for the gaseous phase is set using a Pope spectrum (Pope, 2000). The initial parameters of the spectrum are  $C = 1.5$ ,  $\beta = 5.2$  and  $p_0 = 4$ ,  $c_L = 0.019$ ,  $c_\eta = 0.051$ . All the values of the variables presented in this work are dimensionless and the normalizing Reynolds number is  $Re_0 = u_{ref}L_{ref}/\nu_f = 10^3$ .

The turbulent characteristics of the decaying HIT are given in Table 2 for initial time, injection time and final time. It shows the mean turbulent kinetic energy  $e$ , the dissipation  $\epsilon$ , the Kolmogorov time and length scales ( $\tau_k$  and  $\eta$ ), the Eulerian eddy turnover time  $\tau_f$ , the longitudinal integral length scale  $L_{11}$ , and the turbulent Reynolds number  $Re = u_{rms}L_{11}/\nu_f$ , where  $u_{rms} = \sqrt{2/3e}$  is the gas velocity fluctuations. The energy spectrum is plotted for the corresponding times in Fig. 1. Adequate resolution of statistics is verified with the parameter  $\kappa_{max}\eta = 2\pi/L \times N_g/2\eta = 2.9 \geq 1$ . Comparison of different mesh resolutions is also provided in Appendix B and a good agreement is found between them.

time	$e$	$\epsilon$	$\tau_k$	$\eta$	$\tau_f$	$L_{11}$	$Re$
$t_0$	0.015	0.0089	0.335	0.018	2.11	0.21	21.13
$t_{inj} = 3$	0.054	0.0014	0.854	0.029	4.55	0.27	16.45
$t_f = 6$	0.003	0.00052	1.38	0.037	6.95	0.31	13.47

**Table 2:** Turbulence properties of the HIT



**Figure 1:** Energy spectra at initial time, injection time and final time

To evaluate turbulence modulation by particles, statistical quantities and spectrum of energy are studied. The time-evolution equation of turbulent kinetic energy  $e(t)$  is obtained by multiplying fluid momentum equation by  $u_{f,j}$  and ensemble averaging. The homogeneous isotropic field allows us to use instead the spatial mean  $\langle \cdot \rangle$  previously introduced. It is numerically implemented as the discrete average over all the cells in the domain.

$$\frac{de(t)}{dt} = -\epsilon(t) + \psi_p(t) \quad (8)$$

where  $\epsilon(t) = 2\nu_f \langle S_{ij} S_{ij} \rangle$  is the viscous dissipation rate of  $e(t)$  with  $S_{ij} = \frac{1}{2} \left( \frac{\partial u_{f,i}}{\partial x_j} + \frac{\partial u_{f,j}}{\partial x_i} \right)$  and  $\nu_f$  is the dimensionless kinematic viscosity.  $\psi_p(t)$  represents the energy rate of change due to the particles drag force:

$$\psi_p(t) = \frac{\phi}{\tau_p n_0} \left\langle n(\mathbf{x}, t) u_{f,i}(\mathbf{x}, t) [\tilde{v}_{p,i}(\mathbf{x}, t) - \tilde{u}_{f@p,i}(\mathbf{x}, t)] \right\rangle \quad (9)$$

Performing the Fourier transform of the fluid momentum equation, we obtain the

equation for the energy spectrum  $E(\kappa)$ :

$$\frac{dE(\kappa, t)}{dt} = T(\kappa, t) - D(\kappa, t) + \Psi_p(\kappa, t) \quad (10)$$

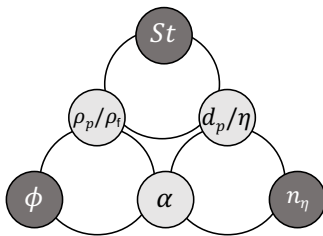
where the spectral dissipation rate is  $D(\kappa) = 2\nu_f\kappa^2E(\kappa)$  and  $T(\kappa)$  is the spectral energy transfer rate. The fluid-particle energy interaction term  $\Psi_p(\kappa)$  produced by particles is responsible for the modulation in the turbulence energy spectrum.

## 2.2. Parameter set for particles

The particles are injected after approximately one eddy turnover time to ensure that natural turbulence is established. At injection time, the particle locations are randomly drawn in the domain, and the particle velocities are set equal to the ones of gas phase at the particle locations. The simulation is run under one-way coupling during approximately one eddy turn over time to thermalize the particles. Then the two-way coupling is activated and the evolution of the turbulence spectrum is analyzed. This delay for the activation of the two-way coupling allows the influence of the particles to be studied once they have naturally segregated. This removes an inconvenient transitional regime observed otherwise, already mentioned by Ferrante and Elghobashi (2003), especially visible for particles with large Stokes.

Regarding some properties of the turbulent flow, dimensionless numbers can be derived, considering fluid density  $\rho_f$ , Kolmogorov time  $\tau_k = (\nu_f/\epsilon)^{1/2}$  and length scale  $\eta = (\nu_f^3/\epsilon)^{1/4}$ . This yields the ratio of the characteristic time of a particle and a turbulence time scale, commonly referred to as the Stokes number  $St = \tau_p/\tau_k$ , the ratio of the diameter of particles and Kolmogorov length scale  $d_p/\eta$  and the dimensionless particle number density, introduced by Poelma et al. (2007), noted  $n_\eta = n_0\eta^3$ , that can be interpreted as the number of particles per Kolmogorov eddy. Volume fraction  $\alpha$ , mass loading  $\phi$  and density ratio can also be derived. All those parameters are related to each other in Fig. 2.

Given a fluid and turbulence properties, only three fundamental units are present: time, mass and length. According to the II-theorem, the system is describable by only three dimensionless parameters of diagram 2, each of which must belong to a different



**Figure 2:** Controlling non-dimensional parameters for particles in turbulence.

”group” (symbolized with the circles in the background of Fig. 2).

The reader can re-examine previous publications with this diagram in mind. Table 1 shows the parameters that were fixed and changed between their different simulations. The parameters in bold font were those identified by the authors as responsible for turbulence modulation. The only consistent and exhaustive study of a given triplet was completed by Elghobashi et al. (1994) who successively observed the separate influence of  $\tau_p$ ,  $\alpha$  and  $d_p$ . However, the use of computational particles to represent several real particles ( $M_r/M_c = 100$ ) can mimic the characteristics of an heterogeneous disperse phase, though aiming at representing a highly-concentrated one (high ”real” particle number density but low ”computational” particle number density). As already noticed by Boivin et al. (1998), neither simulations of Squires and Eaton (1990); Elghobashi et al. (1994) nor their own calculations met the condition of  $n_\eta \gg 1$ , required for correspondence between computational and actual particles. Therefore, only ”real” particles ( $M_r/M_c = 1$ ) are used in our study.

Our choice of description for the disperse phase is represented by the darkest triplet in Fig. 2. The choice of these three parameters was made in view of the proposed form of the interaction term. Indeed, in Eq. 9, mass loading is a factor as well as the inverse of the relaxation time of the particles. We therefore naturally wanted to be able to study the influence of each of these terms in modifying turbulence.

For the description of the system, we see in Fig. 2 that the third parameter can be the volume fraction, the particle diameter or the particle number density. From a

	$St(t_{inj})$	$\phi$	$n_\eta$
	[0.5, 1, 2, 4, 8]	[0, 0.1, 0.2, 0.3]	[0.03, 0.3, 3]
Fig. 3, 17, 21	1	0.001	$2.7 \times 2^j, j = -15, \dots, 0$

**Table 3:** Set of parameters for particles

modeling point of view, we have already seen that the number of particles plays a role in the description of the disperse phase in single-phase flows (Vié et al., 2016). We will see through this work that at fixed Stokes and mass loading, particle distribution in space is essential to quantify the impact on the gaseous phase.

In some of previous works such as those of Druzhinin and Elghobashi (1999) or Druzhinin (2001), particle field has been considered as perfectly homogeneous when  $St \ll 1$ . This assumption was justified by considering that in the case of microparticles the preferential concentration is negligible. However, if particle number density is not large enough, the disperse phase cannot be considered as homogeneous even though the distribution of particles is uniform in the domain. One of the aim of the present work is to give a criterion on particle number density to determine what is the appropriate mean particle number density to consider the two-way exchanges as independent of this parameter.

In the present work, we apply direct numerical simulations to investigate turbulence modulation by inertial particles in decaying isotropic turbulence. Parameters of the disperse phase were successively varied to provide data on modulation of turbulence features and energy spectra according to Table 3. In order to cover the entire parameters space, the exhaustive study of the three selected parameters is carried out according to the parameter values in the first line of Table 3. To emphasize the role played by the particle number density parameter, another set of simulations is performed, with a very large range of values for  $n_\eta$ . To satisfy the assumptions of sub-Kolmogorov particles and dilute regime, the mass fraction is set at a sufficiently low value  $\phi = 0.001$ .

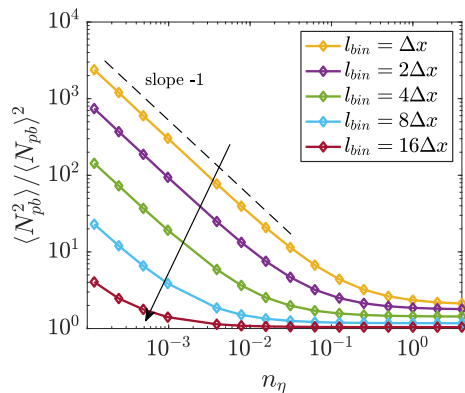
### 3. Defining a measure of disperse phase heterogeneity

In turbulent flows, preferential concentration of particles is a major aspect that can strongly lead the physics (see ? for example). In the literature, several methods have been proposed to measure preferential concentration, and an exhaustive review is proposed by Monchaux et al. (2012). However, preferential concentration is not the only source of phase heterogeneity. Actually, when particle concentration is not high enough, the particulate phase cannot be seen as a continuum, and must therefore be considered as a set of individual particles, and this can have an impact on physics (see for instance Zamansky et al. (2016)). This introduces an additional level of heterogeneity. Here we thus define the heterogeneity of the disperse phase as the combination of the preferential concentration, consequence of the interactions between particles and turbulence, and the lack of continuum, consequence of large particle interspace. In the following, we propose methods that permit to separate both sources, and we also propose a way to identify isolated particles.

#### 3.1. Measurement of preferential concentration

A classical tool to quantify preferential concentration is the PDF of particle number density based on bin counting, which depends on the bin size, as demonstrated by Monchaux et al. (2012) and Hogan and Cuzzi (2001). A possible index to quantify the preferential concentration is the normalized variance of the number density field  $\langle N_{pb}^2 \rangle / \langle N_{pb} \rangle^2$ , with  $N_{pb}$  being the number of particles per bin. Fig. 3 not only confirms the dependency of the measure with the bin size, but also highlights its dependency on the particle number density  $n_\eta$ . For a given bin size, the normalized variance converges when increasing the number of particles. For sufficiently high particle number densities, the statistical sampling becomes redundant and saturated and increasing the number of particles does not add any information in the measure. Moreover, the threshold of convergence depends on the bin size: smaller bins require a higher particle number density to be completely sampled.

Another solution proposed in the literature is the use of Voronoï diagrams based on the Lagrangian point-particle cloud. The local particle concentration is the inverse



**Figure 3:** Evolution of preferential concentration with particle number density for different bin sizes (the arrow shows the increase in bin size). Parameters displayed in Table 3.

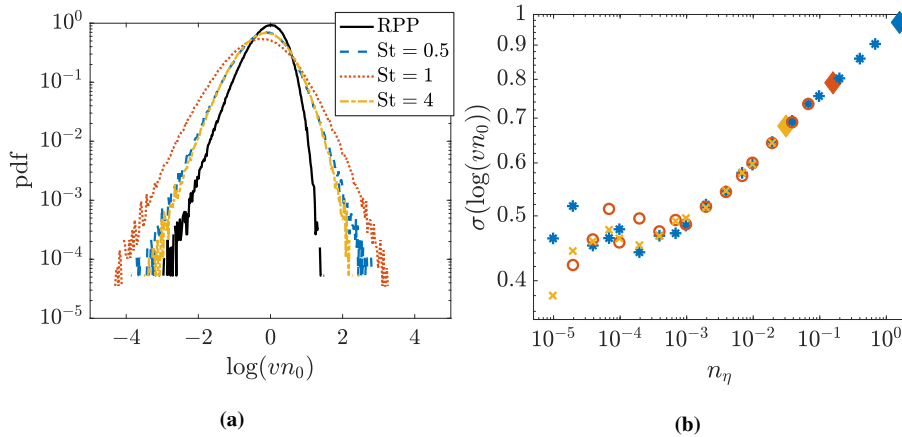
of the volume of Voronoï cells and unlike other segregation calculation methods such as bin counting, they do not depend on the size of the box arbitrarily chosen. A direct measure for the preferential concentration is the standard deviation of Voronoï volume distributions: when clusters and vacuum regions are formed, the tails of the distributions are enhanced and the standard deviation increases.

Figure 4a shows the distribution of the normalized Voronoï volumes normalized by the average particle density<sup>1</sup>, introduced by Monchaux et al. (2010). Three one-way coupled simulations are compared with different Stokes numbers and particle number densities at final time. Figure 4a also shows the distribution generated by a Random Poisson Process (RPP), which corresponds to the perfectly homogeneous case. For all three cases, the standard deviation is greater than for the Random Poisson Process, and it is maximal for a Stokes close to unity, when the highest preferential concentration occurs.

In Fig. 4b, we show the standard deviation of the Voronoï volume distribution for three original simulations with different particle number densities:  $n_\eta = 0.03, 0.15, 1.5$ , respectively the yellow, red and blue diamonds. Similar to the bin counting method,

<sup>1</sup>We recall that the average particle density is independent of the spatial organization of particles.



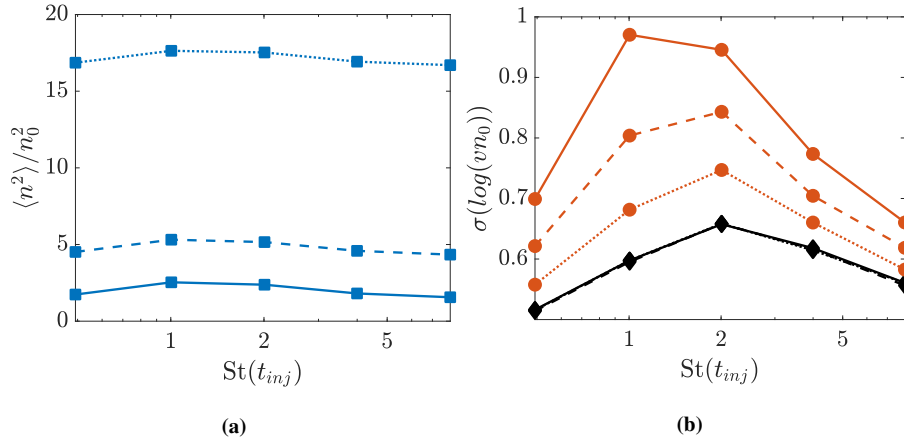


**Figure 4:** (a) PDF of normalized Voronoi volumes. (b) Evolution of the standard deviation of the PDF with the number of particles in simulations, for successive depletion in post-processing.

this measure also depends on the particle number density, and thus does not differentiate the source of heterogeneity between preferential concentration and the lack of continuum.

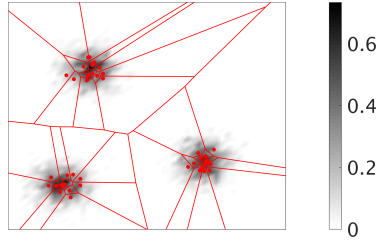
Here we suggest another strategy based on the artificial depletion of the particulate field: before post-processing, we remove particles randomly and we perform the Voronoi analysis on the depleted field. In Fig. 4b (blue stars, red circles and yellow crosses), we show that when the original simulations are artificially depleted, the standard deviation is perfectly scaled as soon as the number of particles is large enough. Therefore, to compare preferential concentration between simulations with different number of particles, we can artificially deplete the highest concentrated simulation until we obtain the same number of particles, as long as the number of particles is large enough to consider the remaining sample significant, when  $n_\eta \gtrsim 10^{-3}$  in our simulations. Below this limit, the depletion strategy is not accurate anymore because of the high sensitivity of the measure to the exact location of the particles.

To summarize, we compare the different measures of preferential concentration introduced above in Fig. 5, for several Stokes numbers. The bin counting method based on the smallest bins ( $l_{bin} = \Delta x$ ) reveals a strong statistical bias that can mask



**Figure 5:** Comparison of preferential concentration for one-way coupled simulations. Dotted lines ( $\cdots$ ):  $n_\eta = 0.03$ , dashed lines ( $--$ ):  $n_\eta = 0.15$  and solid lines ( $—$ ):  $n_\eta = 1.5$ . (a) Bin counting method; (b) Standard deviation of normalized Voronoi PDF before (red lines) and after (black lines) depletion in post-processing.

the preferential concentration of particles for very low particle number densities: the Stokes dependency is not evident for the dotted curve in Fig. 5a. This is corrected in the measure introduced by Monchaux, plotted in red in Fig. 5b. Even for very low particle number densities, the Voronoi diagrams are well defined and the shape of the correct dependency on Stokes number is captured. However, there is still the statistical bias due to the mean particle number density. The black lines represents the new measure we introduced. The scaling of those black curves is consistent with the fact that the same physics rules the preferential concentration, and that the only difference between the red curves is due to the additional sampling. Note that the value of the depleted measure still contains the effect of particle number density because it depends on the reference  $n_\eta$  chosen, but it is now independent of the particle number density of the original simulation. This quantifies the tendency for particles to gather in specific regions of the fluid.

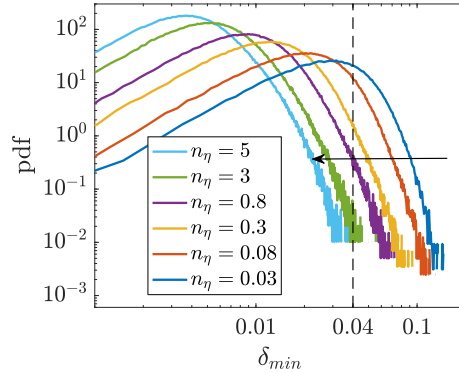


**Figure 6:** 2D Voronoi cells superimposed with particle number density field

### 3.2. Identification of isolated particles

Voronoi cells produce a partition of the domain and thus, even in a regime where all particles are visibly part of a well-converged cluster as in the schematic example of Fig. 6, the cells of particles located at the border of the high density area will include the vacuum domain separating the other clusters. From the definition proposed by Monchaux et al. (2010), those specific particles are therefore not part of any clusters. However, we would like to include them in the cluster given that they are located in the high-density area. On the other hand, we would like to identify if particles are completely isolated from a cluster, and Voronoi volumes fails to provide this information because a large cell volume does not necessarily mean that the associated particle is in a void region. This is why we are considering a different distribution than the Voronoi volumes to avoid this eventuality.

Let us introduce the minimum interparticle distance  $\delta_{min}$ , defined for each particle as the distance between the particle and its closest neighbor. Thus, even for particles on the boundary of a cluster, the minimum distance is small enough to consider that those particles belong to it, while the Voronoi criterion reflects the fact that they belong a vacuum region. The distributions of minimum interparticle distances is given in Fig. 7 for several particle number densities. Naturally, an increase in the particle number density results in a shift of the distribution towards lower values of interparticle distances.



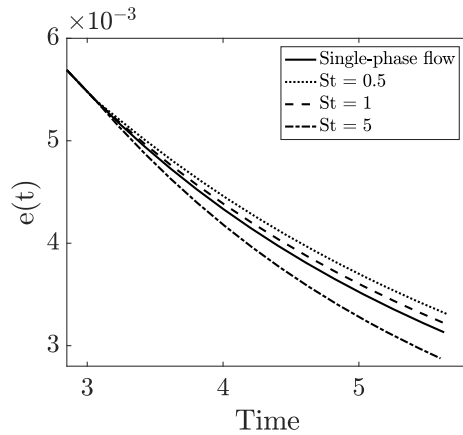
**Figure 7:** Probability density function of minimum interparticle distance for simulation with  $St = 0.45$  and  $\phi = 0.3$  at  $t_f = 6$ . Dotted line represents  $2\Delta x$ .

### 3.3. Summary of proposed measures

We have introduced several measure of particle concentration. We have verified that the bin counting measure of segregation converges with the number of particles, and that particle preferential concentration can be compared between simulations with different number densities using the method of depletion and volume Voronoï PDF. We will therefore use the bin counting method to estimate the convergence of exchanges between particles and fluids at a given scale, and the volume Voronoï PDF will be helpful to compare particle preferential concentration in two-way coupled simulations in section 4.3.1. The minimum interparticle distance gives another characterization of the heterogeneity of the particulate phase, by allowing to identify isolated particles with large interparticle distances.

## 4. Results

An overview of the evolution of statistical quantities and spectra is presented in this section according to the three parameters  $St$ ,  $\phi$  and  $n_\eta$ . The results already observed in the literature for the influence of Stokes number and mass loading are retrieved. Focus is on the role played by the particle number density, and the importance of taking it into consideration for a heterogeneous disperse phase.

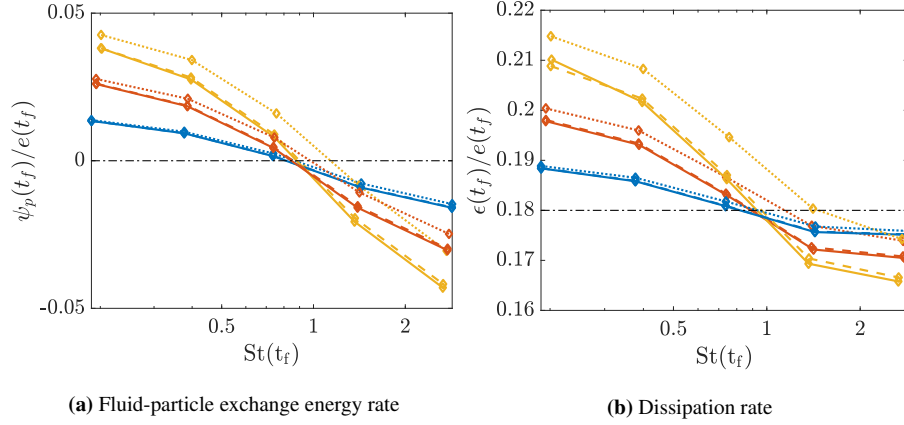


**Figure 8:** Turbulent kinetic energy and decay rate evolution for  $\phi = 0.3$  and a highly-concentrated disperse phase. Stokes number are based on  $\tau_k(t = t_{inj})$

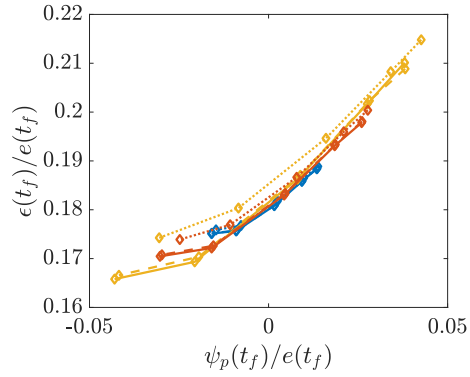
#### 4.1. Two-way interaction energy rate

The existing literature has agreed that there is a criterion for determining whether turbulence will be increased or decreased by the presence of particles. While some studies propose a diameter ratio on a turbulence scale, others have observed the importance of the role played by the Stokes number based on Kolmogorov time scale. Ferrante and Elghobashi (2003) suggested that the critical Stokes (based on the Kolmogorov time scale at injection time) is in the order of 0.25, and therefore name these particles as "ghosts" because of their limited influence on the total energy change of the turbulence. Figure 8 shows similar results: the Stokes number does play a role in the modulation of the kinetic energy of the fluid, with a tendency to slow down the rate of energy decrease for low Stokes, and to increase it for more inertial particles. The evolution equation of this decay rate (Eq. 9) is related to the dissipation term  $-\epsilon(t)$ , to which is added the energy rate of change due to particle drag force  $\psi_p(t)$ .

Figure 9 describes the evolution of the two components of the decay rate: the fluid-particle coupling energy rate (Fig. 9a) and the dissipation rate (Fig. 9b) at a given time  $t_f = 6$  and as a function of the Stokes number. Both are normalized by the total energy budget of the carrier phase  $e(t_f)$ . The two energy rates have very similar behaviors,



**Figure 9:** (a) Normalized fluid-particle exchange energy rate. (b) Normalized dissipation rate versus Stokes number at time  $t_f = 6$ . Lines blue:  $\phi = 0.1$ , red:  $\phi = 0.2$ , yellow:  $\phi = 0.3$ , —:  $n_\eta = 3$ , ---:  $n_\eta = 0.3$ , .....:  $n_\eta = 0.03$ . The black dash-dotted line stands for the single-phase flow.



**Figure 10:** Normalized dissipation rate  $\epsilon/e$  as a function of  $\psi_p/e$ . at time  $t_f = 6$ . Lines blue:  $\phi = 0.1$ , red:  $\phi = 0.2$ , yellow:  $\phi = 0.3$ .

and the strain rate being only a function of the fluid, we deduce that fluid dissipation is closely related to the fluid-particle energy rate. This correspondence is clearly visible in Fig. 10 which groups the fluid dissipation values according to those of the fluid-particle exchange term. Moreover, the change in dissipation relative to the one for single-phase flow is smaller than the source term  $\psi_p$ . Therefore, we will mainly focus on the two-way interaction energy rate and consider the dissipation as a consequence of this term.

We measure a change in the sign of  $\psi_p$  around Stokes number close to unity<sup>2</sup> in Fig. 9a. In the case of  $St < 1$ , the fluid-particle coupling energy rate  $\psi_p$  is positive, because the fluid-particle correlation along the particles paths  $\langle u_{f,i}(\mathbf{x}, t) \tilde{v}_{p,i}(\mathbf{x}, t) \rangle$  is larger than the autocorrelation of the fluid  $\langle u_{f,i}(\mathbf{x}, t) \tilde{u}_{f@p,i}(\mathbf{x}, t) \rangle$  (Ferrante and Elghobashi, 2003). With the inverse coupling, particle energy is given to the fluid resulting in an attenuation of the energy decay rate.

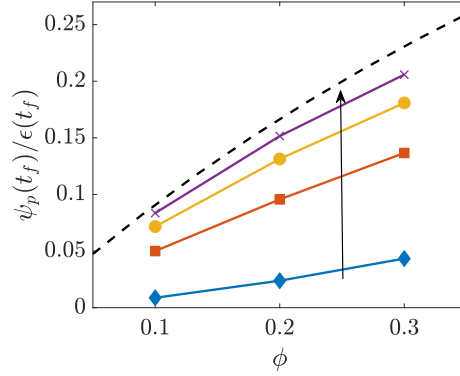
For Stokes numbers close to unity, particles are ejected from the large-vorticity cores but remain in their periphery. Even though fluid-particle energy rate is close to zero, the concentration of particles in those peripheric areas of vortices increases the dissipation.

Conversely, when the inertia of the particles increases, the fluid-particle coupling energy rate becomes negative due to a decorrelation between the velocities of the fluid and the particles. Inertial particles escape from their initial vortices and "cross" the trajectories of fluid points. Accordingly,  $\psi_p$  becomes negative and thus enhances the decay rate of turbulent kinetic energy.

In the scalar limit (for microparticles, i.e.  $St \ll 1$ ), the particle distribution is relatively uniform and particles behave like fluid-tracers. They are not ejected from the vortex cores and they retain their kinetic energy longer than the surrounding fluid. This is called "dusty gas", a phenomenon already described by Saffman (1962) and quantified analytically by Druzhinin (2001). The zeroth-order solution of the two-way

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<sup>2</sup>The Stokes number calculated in our study is based on Kolmogorov scale at the measuring time  $t_f$ , and not the injection time as it is defined by Ferrante and Elghobashi (2003)



**Figure 11:** Fluid-particle coupling energy rate normalized by dissipation rate as a function of mass loading. The arrow shows the decrease in Stokes number:  $St \in [2, 1, 0.5, 0.15]$ . The dotted line is the asymptotic limit analytically predicted.

coupling source term is in the form:

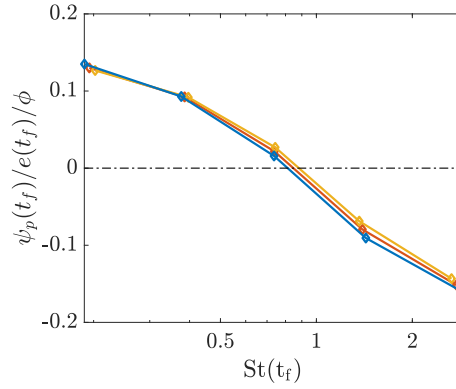
$$\psi_p(t) = \frac{\phi}{1 + \phi} \epsilon(t) + O(St) \quad (11)$$

This asymptotic behavior is retrieved in Fig. 11.

As expected, an increase in mass loading produces a more significant fluid-particle coupling term. Figure 12 suggests that a normalization by  $\phi$  yields a scaling independent of mass loading. Thus, at high Stokes, an increase in mass loading enhances the suppression of kinetic energy. On the contrary, at low Stokes,  $\psi_p$  remains positive, and its absolute value increases, which slows down the natural decrease in the turbulent kinetic energy of the fluid. Physically, the particles with low Stokes follow the fluid particles and thus uniformly charge the vortices, which therefore retain their vorticity longer.

Finally, Fig. 9a shows that the particle number density  $n_\eta$  influences the two-way interaction energy rate, especially when the mass loading  $\phi$  is large. Figure 13, which shows the evolution of the normalized fluid-particle energy rate as a function of the particle number density, confirms that an heterogeneous disperse phase enhances the fluid-particle exchange term contribution. We also plotted on the same figure the seg-



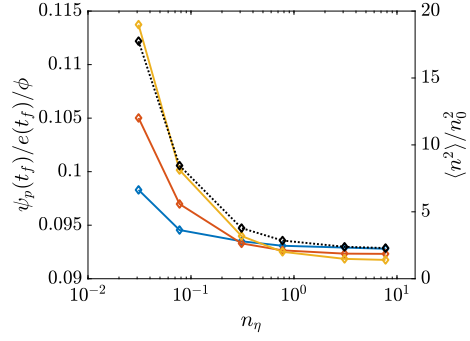


**Figure 12:** Fluid-particle coupling energy rate normalized by mass loading. Lines blue:  $\phi = 0.1$ , red:  $\phi = 0.2$ , yellow:  $\phi = 0.3$ .

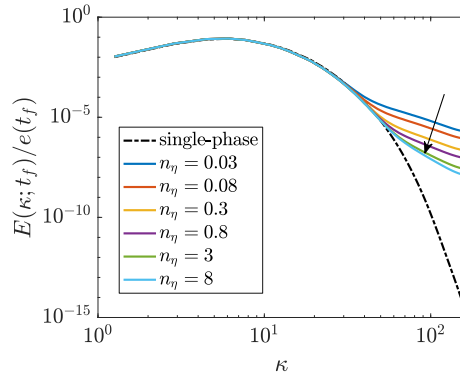
regation (dotted line) measured with size bins corresponding to the smallest resolved scales. The exchange terms and the segregation show similar trends, especially regarding the asymptotic behavior already observed in section 3 that is reached for  $n_\eta \gg 1$ , which is consistent with the idea that sampling becomes statistically significant for a large number of particles per bins of size  $\eta^3$ . A similar statistical convergence was also observed and quantified by Vié et al. (2016) for one-way coupled flows. The asymptotic convergence of the disperse phase segregation with particle number density naturally leads to an asymptotic value for the fluid-particle exchange energy rate as well. We call this regime the highly-concentrated regime: the interactions between fluid and particles are independent on particle number density for  $n_\eta \gg 1$ . In section 4.3.1, we will verify if this convergence is solely a statistical effect (Law of Large Numbers) or related to a modification of the preferential concentration zones.

#### 4.2. Spectral space analysis of two-way coupling energy rate

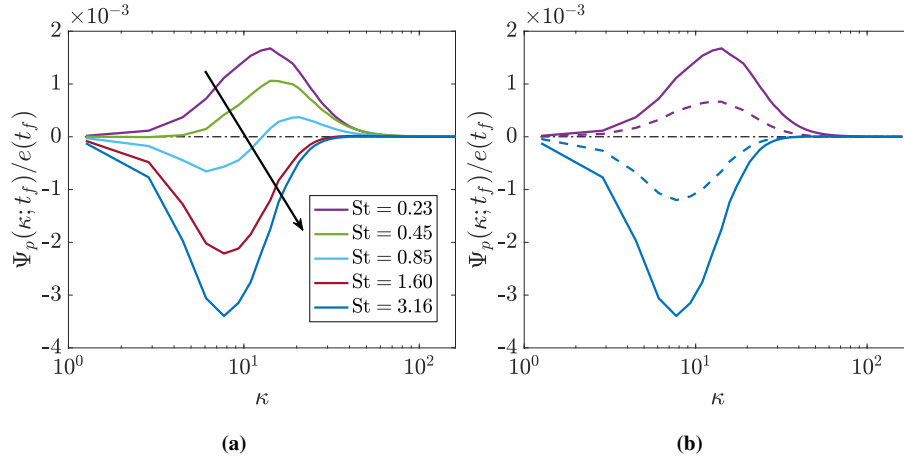
The consequence on the coupling can be further examined by taking the evolution of the energy and forcing spectra. As already observed by Ferrante and Elghobashi (2003), even if the change in the total energy budget is not affected by the presence of small particles (in the case of ghost particles), it does not necessarily imply that the distribution of this energy in the different scales is uniformly zero.



**Figure 13:** Solid lines (—) : fluid-particle coupling energy rate and dotted line (·····) : segregation as a function of particle number density for  $St = 0.4$  at  $t_f = 6$  (respectively left and right axis). Lines blue:  $\phi = 0.1$ , red:  $\phi = 0.2$ , yellow:  $\phi = 0.3$ .



**Figure 14:** Energy spectrum at  $t = 6$  for  $\phi = 0.3$  and  $St = 1.6$ . The arrow shows the increase in the particle number density. The dash-dotted line stands for the single-phase flow spectrum.



**Figure 15:** (a) Influence of Stokes number and (b) mass loading on  $\Psi_p$  spectrum at  $t_f = 6$  for  $n_\eta = 3$ . solid line (—):  $\phi = 0.3$ , dashed line (- -):  $\phi = 0.1$

In Fig. 14, the turbulence spectrum is plotted at time  $t = 6$  for cases without particles, and in the two-way coupled cases for a mass loading of 0.3, a final Stokes number  $St(t_f) = 1.6$ , and six different values of mean particle number densities. The presence of particles enhances the energy at small scales while decreasing the energy at large scales, the overall turbulent kinetic energy being reduced because of the promoted turbulent dissipation. Furthermore, as the particle number density is increased, the spectrum tends to a limit one which corresponds to the highly-concentrated regime.

The fluid-particle interaction spectrum has been extensively studied in the literature. In particular, Ferrante and Elghobashi (2003) compared  $\Psi_p(\kappa)$  for different Stokes number and found similar results. Figure 15a shows that for particles with small Stokes (microparticles),  $\Psi_p(\kappa)$  is positive at almost all wavelengths and thus produces a positive contribution to the decay rate  $\partial E(\kappa)/\partial t$ . On the other hand, the term is negative at almost all wavelengths for larger Stokes. For intermediate and large Stokes,  $\Psi_p(\kappa)$  remains positive for large  $\kappa$  while a negative peak appears in the spectrum for small  $\kappa$ . It can be assumed that in the neighborhood of the particle, the fluid particles "follow" the inertial particle, thus producing a local correlation of particle velocity with the velocity of the surrounding fluid. This results in a positive interaction

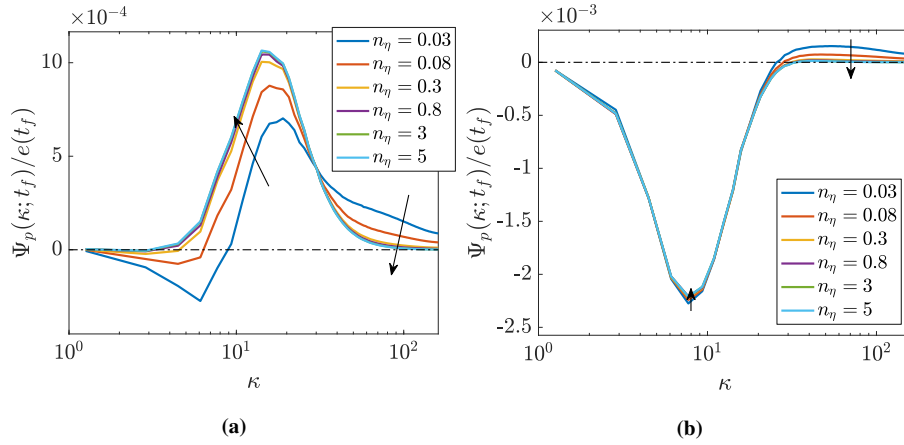
at high  $\kappa$  on the  $\Psi_p$  spectrum. Figure 15b shows the spectral fluid-particle interaction for two different Stokes and two different mass loading. As mentioned in section 4.1, the scaling between spectra with same Stokes but different mass loading is close to the ratio of mass loading, but because of the non-linearity, we do not expect such scaling for higher mass loading.

Previous results show that a low particle number density results in an increase in the fluid-particle interaction energy rate  $\psi_p(t)$ , especially when the mass loading is high. Let us study the spectrum of this exchange term to understand at what scales the interactions between particles and fluid are located and how the distribution of mass loading can modify the fluid energy. A high particle number density produces a highly-concentrated particle number field in which each particle is light and takes part in a collective cluster of particles. On the contrary, a low particle number density generates a heterogeneous particle concentration field and therefore individual particles are more isolated and heavy.

We can see in Figs. 16a and 16b that a heterogeneous disperse phase ( $n_\eta = 0.03$ ) produces a larger  $\Psi_p(\kappa)$  at small scales than a highly-concentrated one ( $n_\eta = 5$ ). However, for particles with small Stokes in Fig. 16a, this effect is reversed at large scales of the fluid and the highly-concentrated disperse phase produces a stronger source term. On the other hand, for particles with higher Stokes in Fig. 16b, the negative peak at large scales is enhanced by the collective effect of clustered particles. In both cases, at larger scales, the fluid-particle exchange of the heterogeneous disperse phase is reduced (in absolute value) compared to the highly-concentrated one.

### 4.3. Particle field heterogeneity

For a physical intuition of the interpretation of the spectra in section 4.2, the spatial distribution of the corresponding fields before the Fourier transform can be examined. Figure 17 compares the spatial distribution of the local two-way interaction energy rate  $\tilde{\psi}_p(\mathbf{x}, t) = \mathbf{u}_f(\mathbf{x}, t)\mathbf{f}(\mathbf{x}, t)/\rho_f$ , with superimposed particles in a part of the flow do-



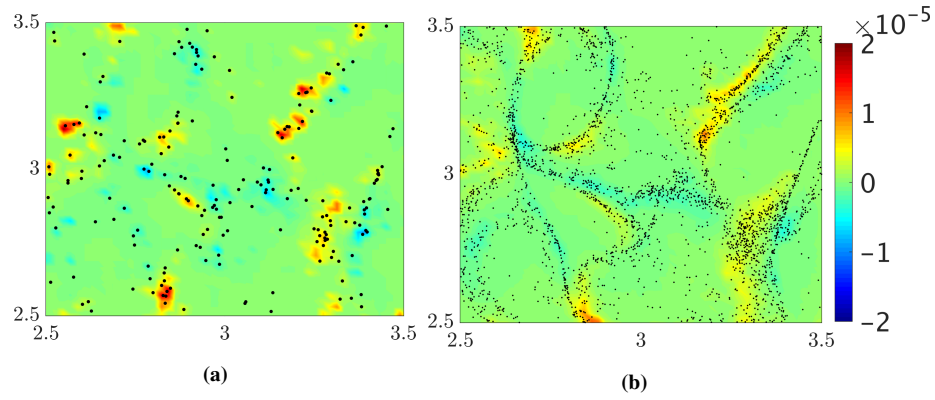
**Figure 16:** Spectral fluid-particle interaction plotted for different particle number densities  $n_\eta$  and fixed  $\phi = 0.3$ . (a)  $St = 0.45$ ; (b)  $St = 1.60$

main at time  $t = 6$ . Particles parameters were set to the same Stokes number  $St = 1$ , and global mass loading  $\phi = 0.001$ , but different particle number densities. Figure 17a shows that each isolated particle produces a localized contribution to the two-way interaction term, and therefore the two-way interaction field is more heterogeneous than for the case with higher  $n_\eta$ , accordingly to the corresponding particle concentration field. By increasing the particle number density  $n_\eta$  without changing the total mass  $\phi$  nor the behavior of each particle defined by  $St$ , see Fig. 17b, each particle produces a smaller individual effect on the fluid. On the other hand, the collective effect of segregated particles results in a smoother and well-distributed two-way interaction field.

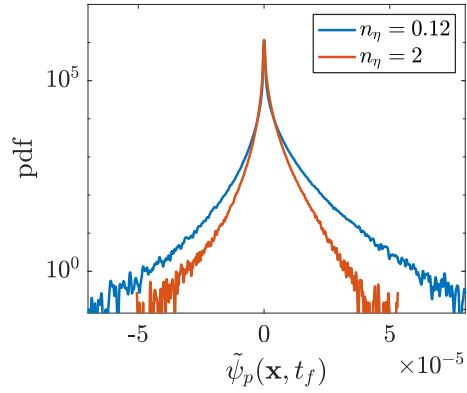
The probability distribution function of the corresponding spatial two-way interaction terms is plotted in fig. 18, and the reduction of the tails indicates a better distributed interaction term for highly-concentrated disperse phase.

#### 4.3.1. Preferential concentration

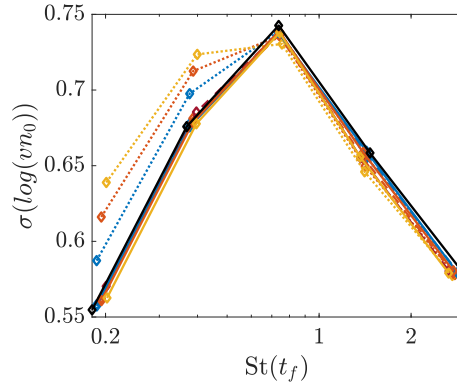
Figure 19 shows the standard deviation of the normalized Voronoï volume distributions for the different configurations. As explained in section 3, the simulations were depleted in post-processing to equalize to the same number of particles in order to be



**Figure 17:** Distribution of two-way interaction energy rate  $\tilde{\psi}_p$  at  $t = 6$  superimposed with particles parametrized by  $\phi = 0.001$  and  $St = 1$ . (a)  $n_\eta = 0.12$  ; (b)  $n_\eta = 2$



**Figure 18:** Distribution of the two-way interaction energy rate field  $\tilde{\psi}_p(\mathbf{x}, t)$  for the heterogeneous and highly-concentrated cases.



**Figure 19:** Comparison of preferential concentration for all simulations. Lines blue:  $\phi = 0.1$ , red:  $\phi = 0.2$ , yellow:  $\phi = 0.3$ , —:  $n_\eta = 3$ , - - -:  $n_\eta = 0.3$ ,  $\cdots$ :  $n_\eta = 0.03$ . The black dash-dotted line stands for the single-phase flow.

able to compare them without statistical bias. The quasi-scaling of those curves is consistent with the fact that the Stokes number based on real time governs the preferential concentration, revealing that the adaptation is faster than the decrease in energy. Only simulations with low particle number density and low Stokes number increase the preferential particle concentration effect. We can conclude that all the two-way coupling effects that we analyze in our simulations are not a consequence of a modification of the clustering.

#### 4.3.2. Collective and isolated regimes

A single particle will interact and exchange energy with the surrounding fluid up to a characteristic distance of  $\delta_i$ , which is directly related to the size of the projection kernel<sup>3</sup>. The source term introduced in the fluid momentum equation is limited to the kernel envelope  $\delta_i$  and we will consider that a particle is "isolated" if it is distant from others of more than  $\delta_i$ . On the contrary, if two particles are closer than this length-scale, their corresponding source terms can be superposed and these two particles form a "cluster".

<sup>3</sup>Using a trilinear projection, we verify that  $\delta_i = \Delta x < \eta$

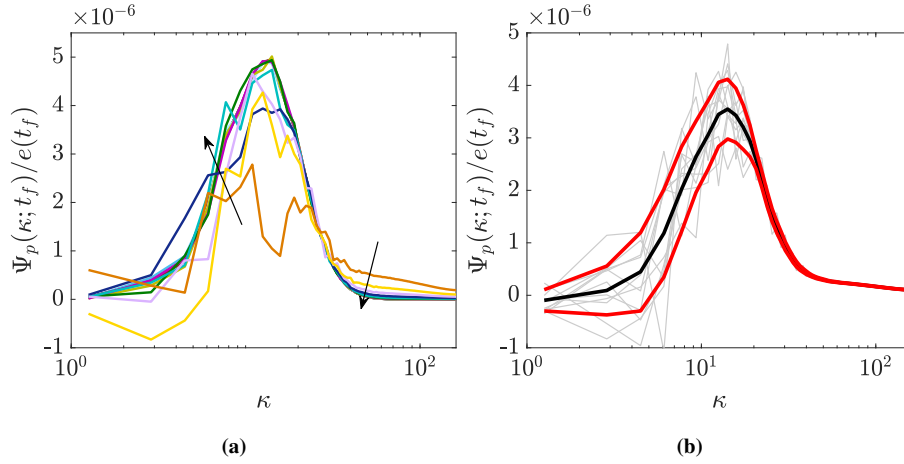
Let us consider the two limit regimes where particles are either all isolated to each other, or all part of a cluster. Those two configurations correspond to the PDF of the minimal interparticle distance being respectively on the right or on the left side of the  $2\delta_i = 2\Delta x$  boundary, see Fig. 7 (dotted line). These limit behaviors are indeed observed in Fig. 16: green and light blue distributions of Fig. 7 are on the left of  $2\delta_i$  and produced in Fig. 16 overlapped spectra, because the particulate phase is already converged and increasing particle number density do not change the interaction spectrum anymore. However, for the other distributions, on the other side of the threshold, one can see in Fig. 16 that the spectra are strongly dependent on particle number density, especially at the smallest scales, the last ones to reach convergence.

Let us explained these limit behaviors. If particles are all isolated from each other, then the particles properties locally determine the amount of energy exchanged with the fluid and the global budget is a statistical average of all the exchanges. Thus, if we modify the properties of this particle, for example by decreasing the particle number density of the simulation while ensuring that we keep isolated particles, then the mass  $m_p$  of the single particle is now larger and the amount of energy transferred will be locally larger. In this regime, the two-way interaction spectrum is highly sensitive to particle number density, especially at the smallest scales of the fluid, where particles inject an energy almost proportional to their mass.

On the contrary, if every particle is part of a cluster, the force exerted by particles on the fluid can be assimilated to a continuous force on the cluster domain. By increasing particle number density but maintaining the mass loading, the total mass and therefore the energy contained in each cluster is unchanged. Therefore, the two-way interaction spectrum is unchanged, this collective regime leads to the two-way limit behavior observed for spectra.

This criterion is very restrictive, those two limit regimes are rarely reached and we propose in the next section an other approach to characterize the transition from the isolated to collective regime, scale by scale.



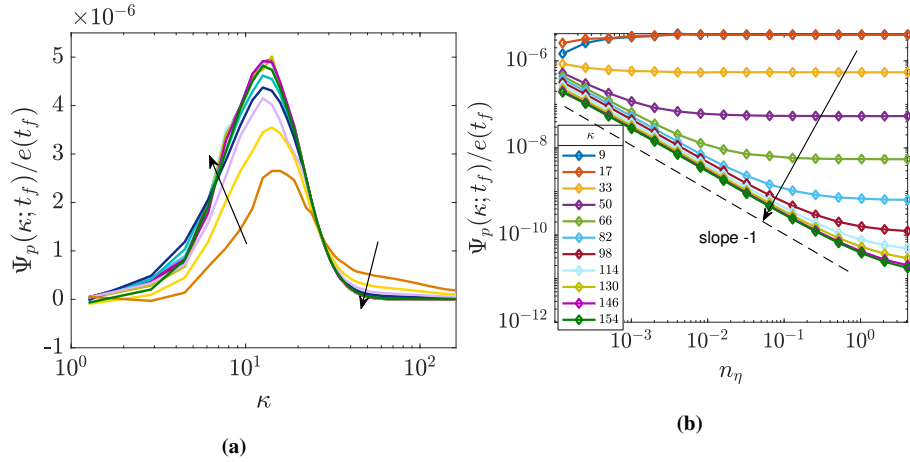


**Figure 20:** (a) Two-way interaction spectra for different particle number densities  $n_\eta = 2.7 \times 2^j$ ,  $j = -15, \dots, 0$ , and fixed  $St = 1$  and  $\phi = 0.001$  (The arrow shows the increase in  $n_\eta$ ). (b) Two-way interaction spectra for 11 realizations of simulation with  $n_\eta = 2.7 \times 2^{-14}$  (grey lines), the mean spectrum (black solid line) and the standard deviation (red solid lines).

#### 4.3.3. Scale by scale convergence

The two-way interaction spectrum indicates for each wavelength the amount of energy introduced into the spectral equation. More precisely, each wave-number  $\kappa_l$  is associated to a physical size  $l = \frac{2\pi}{\kappa_l}$ . Thus, the term  $\Psi_p(\kappa_l)$  specifies the average energy provided by the exchange term in boxes of size  $l$  contained in the domain. Figure 20a shows the interaction spectrum for different particle number densities. For very low particle number densities, the spectrum is noisy at the largest scales due to a lack of statistics available for the corresponding box sizes.

To illustrate the strong variability of the spectrum realizations between different simulations (same parameters of the disperse phase and the gas phase but different initial particle distribution), we reported in Fig. 20b the two-way interaction spectra of several realizations, along with the mean spectrum (black line) and its standard deviation (red lines). The variability between the different realizations is reduced at the smallest scales because one flow realization contains a sufficiently large sample of small eddies to ensure statistical convergence.



**Figure 21:** (a) Two-way interaction spectra averaged between several realizations. (b) Evolution with  $n_\eta$  of the spectral values for different wavenumbers (the arrow indicates increasing wavenumbers).

In the following, to only take into consideration the effect of a representative realization of a highly heterogeneous disperse phase, we consider the average spectrum associated with several realizations (black spectrum). We thus obtain Fig. 21a, identical to Fig. 20a for large  $n_\eta$  but less noisy for small  $n_\eta$ .

In Fig. 21b, we have plotted for several wavelengths the evolution of the spectrum values at those scales when  $n_\eta$  increases.

For each graph in this figure, we observe two very distinct regimes: a first linear zone of slope  $-1$  for low  $n_\eta$ , and a second zone for high  $n_\eta$ , in which the spectrum values are converged and are therefore no longer modified when the particle number density increases. Those regimes are respectively the isolated (linear) and collective (converged) regime introduced before. This scale-by-scale convergence can be correlated with the convergence of the segregation measure defined with bin counting of corresponding sizes in Fig. 3, and is also a consequence of the statistical sampling related to the scale in consideration: the large scales reach their asymptotic value for smaller  $n_\eta$  than small scales, because the number of particles per scale is larger.

## Conclusion

An exhaustive study of the influence of the three parameters describing a monodispersed phase on isotropic homogeneous turbulence has been carried out. Classical results from the literature have been retrieved, in particular the global trends in energy and spectral statistics with the Stokes number and mass loading. The study of the two-way coupling term here normalized by fluid kinetic energy and the use of a Stokes number based on instantaneous Kolmogorov scales have permitted to clearly identify two regimes: a first regime for  $St < 1$  in which particles promote turbulent energy, and a second regime for  $St > 1$  in which particles destroy turbulent energy.

Additionally to the existing literature, the present study has emphasized the influence of the particle number density on the coupling term. First, we ensured with a Voronoï analysis that the structure of turbulence is not strongly modified by the presence of particles: turbulence is sustained or dissipated but particle preferential concentration remains directly correlated to the updated Stokes number.

Numerical simulations have revealed that a highly heterogeneous particulate phase tends to increase the energy transmitted to the fluid. In particular, a spectral analysis showed that isolated particles inject energy at the finest scales while a continuous particulate phase no longer produces energy at these scales but rather at smaller wavelengths. Those two regimes are reflected in the behavior of the energy spectra:

- At "small" scales, the spectrum is strongly dependent on particle number density and behave almost linearly with this parameter: the energy injected by particles is almost proportional to individual particle mass because particles are isolated regarding those specific scales.
- At "large" scales, the spectrum is no longer modified by the number of particles since the sampling is significant enough, all these scales necessarily contain a large number of particles.
- The limits for "small" and "large" scales depend on the mean particle number density.

- If the distribution of minimal interparticle distance is on the left side of  $\eta$ , the spectrum is completely converged: increasing particle number density does not modify the spectrum.

Furthermore, due to the high variability of the spectrum at large scales for low particle concentration, we have highlighted the necessity to construct statistics over several flow-particles realizations.

This study therefore made it possible to determine precisely the conditions of partial or total convergence of the spectrum as a function of the particle number density, and more precisely of the distribution of interparticle distances.

As a conclusion, it must be noted that such regimes, whereas being intrinsically present in Lagrangian point-particle approaches, must be included and modeled when the carrier phase description is given by a reduced description such as Large Eddy Simulation. The use of adapted Lagrangian Stochastic models must be considered. For Eulerian approaches, even with a fully resolved carrier phase, accounting for heterogeneous regime requires new developments and closures at the kinetic level.

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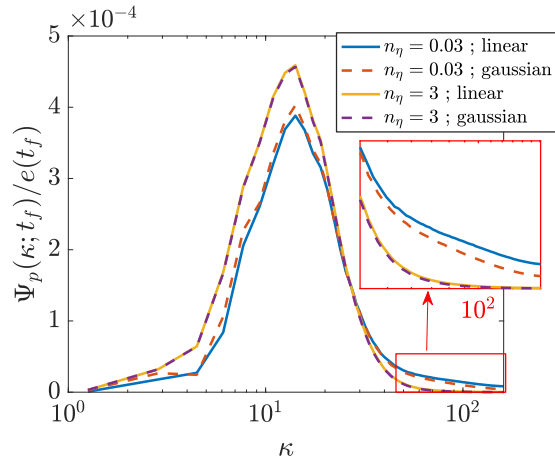
## Appendix A. Impact of the coupling kernel

Let us introduce the threshold  $\delta_i$ , the characteristic size of the domain of influence of a particle on the surrounding fluid. This numerical quantity corresponds to the size of the volume filtering kernel, usually determined to fit the physics. Several works are dedicated to the determination of the parameter  $\delta_i$  for finite size particles (see for instance Maxey and Patel (2001)), the objective being to ensure that the force distributions are completely contained within the interior of the particle. This corresponds in our case to  $\delta_i \leq d_p \leq \eta$ . Knowing that anything under Kolmogorov scales will be immediately dissipated by the fluid, any size of  $\delta_i$  can be chosen under  $\eta$ . In our numerical implementation, we use a gaussian filter with size  $\sigma = \Delta_x/2\sqrt{2\ln(2)}$  such that the full width at half height of the kernel  $\delta_i$  is equal to the grid spacing. This way, the effect of the particle is typically spread out over the 27 nearest cells. Results are compared with the trilinear projection kernel.

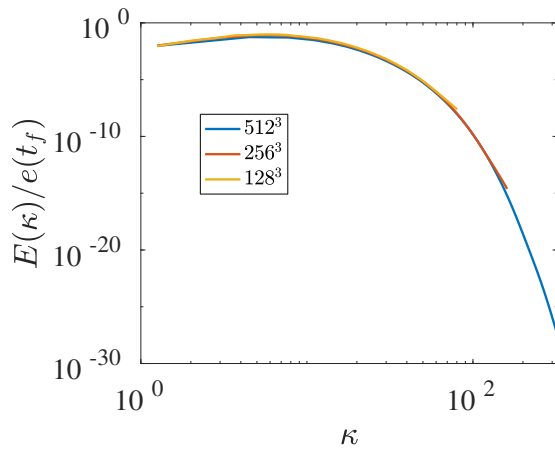
Thus, in Fig. A.22, the comparison of the interaction spectra obtained is consistent with the previous wavelength analysis: for simulations with a large number of particles, statistical convergence is achieved at all scales and thus the kernel change has no impact on the interaction spectrum. On the other hand, at low particle number density, the small scales are less energetic with the Gaussian kernel which spread the energy of the particles at these scales over a larger range of influence  $\delta_i$ . It should also be noted that large scales are then more energetic in this case, since the total interaction energy must be preserved.

## Appendix B. Mesh convergence

We verified the convergence of the spectra for different grid sizes in Fig. B.23. Spectra overlapped in their definition domain, which ensures that the smallest scales are always appropriately resolved. The results presented in this work were obtained using the  $256^3$  grid.



**Figure A.22:** Normalized two-way interaction spectrum with trilinear (solid lines) and gaussian (dashed lines) projection. Two different particle number densities are compared. The inset displays a zoom around the smallest scales.



**Figure B.23:** Comparison of Energy spectrum for different size of meshgrids

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