Investigation and quantification of flow unsteadiness in shock-particle cloud interaction

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Keywords
shock-particle interaction, unsteadiness, vorticity equation, velocity fluctuations

Disciplines
Chemical Engineering | Mechanical Engineering | Mechanics of Materials

Comments

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To be published in: International Journal of Multiphase Flow
DOI to publisher's version: 10.1016/j.ijmultiphaseflow.2018.01.011
INVESTIGATION AND QUANTIFICATION OF FLOW UNSTEADINESS IN SHOCK-PARTICLE CLOUD INTERACTION

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Abstract

This work aims to study the interaction of a shock wave with a cloud of particles to quantify flow unsteadiness and velocity fluctuations using particle-resolved direct numerical simulation (PR-DNS). Three cases are studied, with each case revealing one aspect of the intricate flow phenomena involved in this interaction. The unsteady interaction of a shock wave with a transverse array of particles reveals the origin of unsteadiness under the effect of mutual wave-wave and wave-wake interactions between the particles. In the second case, the interaction of a shock with a particle cloud is studied, with a focus on the interaction of the complex wave system with the vortical structure. A budget analysis of the vorticity equation reveals the sources of strong unsteadiness in the particle cloud. A detailed analysis of the velocity fluctuation and kinetic energy in the fluctuating motion is performed to ascertain the importance of the velocity fluctuations that arise from the strong unsteadiness. An analogous analysis is presented, in the third case, for a gradually-induced flow on the same particle cloud along with a comparison to the shock induced case to assess the impulsive effect of shock on intensity of the fluctuating field statistics.

Key words: shock-particle interaction, unsteadiness, vorticity equation, velocity fluctuations

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1. Introduction

The interaction between shock waves and particles is an important phenomenon in compressible particle-laden flows [1]–[6]. When a shock wave propagates around a particle a complex wave system including regular and irregular shock-wave reflection and diffraction is established [7]–[11].

Shock interaction with a single isolated particle has been studied extensively [9], [10], [12], [13]. In many typical applications, shock waves interact with a cloud or dispersion of particles [14]–[16]. In these processes, depending on the solid phase volume fraction, $\alpha_s$, the flow topology ranges from a very dense gas-solid flow ($\alpha_s \geq 0.5$) during the propagation of the shock wave within the particle cloud to a dilute gas-solid flow ($\alpha_s < 0.01$), at distances far from the source. Between these two extremes ($0.01 < \alpha_s < 0.5$), there exists a dense gas-solid flow regime during early interaction times. A detailed discussion of these three regimes is given by Zhang et al.[17].

The modeling techniques developed for an isolated particle are suitable for dilute particle-laden flows (i.e., with negligible particle volume fraction), but cannot be applied directly in dense particle-laden flows (i.e., with finite particle volume fraction) [8], [9]. With increasing particle volume fraction, the existence of neighboring particles further complicates the interaction between shock waves and particles. In these situations, inter-particle interactions, interactions between particles and reflected or diffracted waves from neighboring particles, and interactions between particles and the wakes of neighboring particles become important.

Much experimental work in the dilute regime has been conducted [18]–[20]. Simulations and theoretical analysis have been applied to predict shock attenuation in this regime [21], [22]. Computational modeling has also shown the capability to capture the gas–solid flow physics in the
very dense regime. For instance, Baer and Nunziato [23] use continuum mixture theory to accurately model the normal shock impingement. However, there is a substantial knowledge gap in gas–solid flows with intermediate particle volume fractions that are roughly equivalent to those found in dense gas–solid flow. Thus, detailed knowledge of the interactions that occur in dense gas–solid flow is required [6], [8], [24], [25].

On the other hand, shock–particle interaction is strongly time-dependent [4], [12], [26]. The particle is subjected to very strong gas acceleration as the shock wave passes over it [25], [27]. Sun et al. [12] and Bredin and Skews [28] presented time-resolved measurements of the force on a stationary particle subjected to a shock wave. The instantaneous force on the particle under such highly unsteady conditions was shown to be much larger than the corresponding quasi-steady force that would have resulted if the change from the quiescent pre-shock state to the uniform post-shock state were to happen very slowly [4], [8]. In particular, the instantaneous force during the passage of the shock wave is reported to be an order of magnitude larger than the steady drag force resulting from the post-shock gas velocity [6]. This clearly highlights the importance of unsteady effects in shock–particle interactions.

The unsteady effects are usually neglected even if strong interactions between compressible flow features and particles are to be expected [17], [29], [30]. However, in some applications, such as in detonations, the large unsteady forces exerted on the particle can cause deformation and breakage. Similarly, intense unsteady heating can cause melting or initiate chemical reactions. There are a limited number of papers that address the influence of unsteady forces on the motion of particles interacting with a shock wave, such as Parmar et al. [13] and Forney et al. [2]. Ling et al. [1], [6], [8] also proposed a model that includes unsteady contributions to particle-fluid interaction force and heat transfer.
Wagner et al. [25] pioneered an experiment to isolate the flow behavior involved in a multiphase shock tube to investigate the unsteady interaction of a shock with a Mach number of 1.67 with a dense particle cloud. Ling et al. [8] developed a one-dimensional phase-averaged point-particle model, including the unsteady momentum coupling forces, to reproduce the experimental results of Wagner et al. [25]. The results highlight the importance of unsteadiness in the shock-particle interaction in the dense gas-solid regime. Although this model appears promising, it is appropriate to question whether all aspects of the experimental flow can be captured using a one-dimensional model that only includes the unsteady momentum coupling forces. Regele et al. [31] took a step forward in revealing the complex phenomena in this interaction and showed that high flow unsteadiness is present in the flow field. They compared the phase averaged results with a 1D model and indicated that the 1D model can characterize the overall steady-state flow behavior but fails to capture unsteady behavior due to the neglect of unsteady terms such as the Reynolds stress. There is also evidence that the Reynolds stress can be important in simple homogeneous incompressible flow in the dense particle-laden regime [32], [33]. In these results, the inter-particle interactions, the interactions between particles and the wakes of neighboring particles play a role. However, the interactions between particles and the reflected or diffracted waves from neighboring particles is absent. Even in the absence of shocks, Mehrabadi et al. [32] showed that the Reynolds stress term is non-negligible and fluctuations in the gas-phase velocity can contribute significantly to the total gas-phase kinetic energy. Furthermore, the authors denote local particle-scale gas-phase velocity fluctuations generated by the presence of particles, larger than the Kolmogorov length scale, as pseudo-turbulent velocity fluctuations. They refer to the kinetic energy associated with these fluctuations as the pseudo-turbulent kinetic energy (PTKE) because these fluctuations can be generated even in laminar gas-solid flow. They show that the PTKE in the fluctuating motion
can be as high as the kinetic energy in the mean flow, especially for systems with higher solid volume fractions. The ratio of PTKE to mean kinetic energy increases with the solid volume fraction and decreases with the mean slip Reynolds number. This provides evidence that the pseudo-turbulent effects play an important role in the dense gas-solid regime. Sun et al. [33] provided evidence that the velocity fluctuations can also result in temperature fluctuations.

Regele et al. [31] showed that velocity fluctuations from shock-particle interactions are more significant and can be on the same order as the mean velocity. However, since the calculations were performed with the Euler equations, additional studies including viscous and thermal diffusion are required to more accurately quantify the magnitude of the velocity fluctuations. These observations along with the experimental results of Wagner et al.[25] indicate that quantification of the unsteadiness and gas-phase velocity fluctuation in the shock-particle cloud interaction is necessary to better understand the flow interaction.

The overarching goal of this paper is to quantify the flow unsteadiness and velocity fluctuations induced by shock waves interacting with particle-clouds and determine their sources. The approach is to perform 2-D simulations of shock waves impacting an array or cloud of particles, where the same Mach number and particle configuration used in Regele et al. [31] is used for consistency. The fully compressible Navier-Stokes equations are solved with a characteristic based volume penalization method [34], which provides a more accurate estimate of the magnitude of these terms than the previous Euler simulations [31]. A transverse array of particles is used to obtain deeper insight into the wave dynamics and unsteady vortex generation on each particle under the mutual wave-wave and wave-wake interaction between the particles. Quantification of the shock-particle cloud interaction highlights the impact of the complex shock dynamics that arise from the effect of neighboring particles on the mean and fluctuating flow field
Finally, in addition to the flow unsteadiness induced by fluid flowing through the particle cloud, the initial interaction of the shock wave with the particle cloud is likely to produce flow unsteadiness itself. It then becomes unclear how to differentiate between unsteadiness that originates from the initial shock wave and vortical motion. In order to distinguish between these two sources, additional simulations of gradually-induced flow over the same particle cloud are performed to remove the impulsive effect of the shock and understand how the impulsive shock dynamics contribute to the unsteadiness and the fluctuating field statistics.

The paper is organized as follows. The mathematical approach and the numerical methods are presented in sections 2 and 3 respectively. The results for a shock wave impacting a transverse array of particles are contained in Section 4 and the results describing the particle cloud behavior are in section 5. Finally, conclusions are drawn in section 6.

2. Mathematical approach

2.1 Governing equations for PR-DNS

In this work the interaction of shock and compression waves with particles are studied where the particles are frozen in place because of the large density ratio between the two phases [31]. In these interactions the smallest scale flow feature, other than the shock thickness, is the boundary layer present near the surface of each particle. The appropriate method to accurately capture these flow features is the Particle-Resolved Direct Numerical Simulation (PR-DNS) methodology in which the flow scales, introduced by the presence of large particles, are resolved [32], [33]. To this end, the fully compressible Navier-Stokes equations are solved to ensure the accuracy of the captured features in the cloud and the wake structure behind the cloud. The non-dimensionalized continuity, momentum and energy equations in conservative form are
\[
\frac{\partial p}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0
\]  

(1)

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re_a} \frac{\partial (\tau_{ij})}{\partial x_j}
\]  

(2)

\[
\frac{\partial (\rho E)}{\partial t} + \frac{\partial ((\rho E + p)u_j)}{\partial x_j} = \frac{1}{Re_a} \frac{\partial (u_i \tau_{ij})}{\partial x_j} + \frac{1}{(\gamma - 1)Re_a Pr} \frac{\partial}{\partial x_j} \left( k \frac{\partial T}{\partial x_j} \right)
\]  

(3)

where the velocity, \( u_i \), is non-dimensionalized by a reference speed of sound \( c_0 \), time (\( t \)) by \( l/c_0 \), total energy (\( E \)) by \( c_0^2 \), density (\( \rho \)) by \( \rho_0 \), pressure (\( p \)) by \( \rho_0 c_0^2 \), viscosity (\( \mu \)) by \( \mu_0 \), thermal conductivity (\( k \)) by \( k_0 \), and temperature (\( T \)) by \( T_0 \). All quantities with subscript “0” denote the reference state, which is the undisturbed gas state. The Prandtl number (\( Pr = \mu c_0 / k_0 \)) is defined as the ratio of the momentum diffusivity to thermal diffusivity. \( Re_a \) is the acoustic Reynolds number determined by the characteristic length scale, \( l \),

\[
Re_a = \frac{\rho_0 c_0 l}{\mu_0}.
\]  

(4)

The non-dimensional equation of state is

\[
p = (\gamma - 1)\rho \left( E - \frac{1}{2} u_i u_i \right).
\]  

(5)

The non-dimensional stress tensor, \( \tau_{ij} \), is expressed

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right),
\]  

(6)

and the temperature is found using a non-dimensionalized ideal gas equation of state

\[
T = \gamma p / \rho
\]  

(7)

with \( \gamma = 1.4 \). The temperature dependence of viscosity, \( \mu \), is assumed to follow Sutherland's law[35]
\[ \mu = \frac{1 + S_1}{T + S_1} T^{1.5} \]  

where \( S_1 \) is Sutherland constant normalized by \( T_0 \) and has the value of 0.4.

### 2.2 Immersed Boundary method

Particle Resolved DNS coupled with immersed boundary methods is a common approach used to study particle scale fluid dynamics [32], [33], [36]–[39]. However, most of these approaches are based on incompressible formulations. Recently, Brown-Dymkoski et al. [34] developed a characteristic-based volume penalization method for compressible flow based on an extension of the Brinkman Penalization Method that allows any arbitrary Dirichlet, Neumann, or Robin-type boundary condition and has been applied to several validation test cases [34] in the Adaptive Wavelet Collocation framework (explained in the next section). In this work, the volume penalization method developed by Brown-Dymkoski et al. [34] is used to impose adiabatic no-slip conditions at particle surfaces. The penalization equations are:

\[ \frac{\partial \rho}{\partial t} = (1 - \chi)RHS - \chi \left( \frac{\rho}{\eta_c} \frac{\partial \rho}{\partial x_k} - \phi \right) \]  

\[ \frac{\partial \rho u_i}{\partial t} = (1 - \chi)RHS - \chi \left[ \frac{1}{\eta_b} \rho (u_i - u_{0i}) + \rho \nu_n \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{u_i}{\eta_c} \left( \frac{\partial \rho}{\partial x_k} - \phi \right) \right] \]  

\[ \frac{\partial \rho E}{\partial t} = (1 - \chi)RHS \]  

\[ - \chi \left[ \frac{1}{\eta_c} \left( \rho \frac{\partial \rho E}{\partial x_k} \right) + \frac{1}{\eta_b} \rho (u_j - u_{0j}) u_j - \frac{1}{\eta_c} \rho u_j n_k \frac{\partial u_j}{\partial x_k} - \rho u_j n_n \frac{\partial^2 u_i}{\partial x_j \partial x_j} \right] \]  

\[- \frac{1}{\eta_c} E \phi - \frac{1}{\eta_c c_p \rho q} \]

where \( \chi \) is a mask function that is unity inside the object and zero outside, RHS indicates the right-hand side of the Navier-Stokes equations, and \( n_k \) is the inward facing surface normal of the object.
The interior of the particles is governed by the penalization terms, while outside the particles, the equations are the same as the Navier-Stokes equations. The velocity $u_{0j}$ is the velocity of the object, which for this work is zero. The parameters $\eta_c$, $\eta_b$, and $\nu_n$ control the accuracy and numerical stability as described in Ref. [34]. In the penalization for $\rho$, the quantity $\phi$ is governed by the equation

$$\frac{\partial \phi}{\partial t} = -\frac{\chi}{\eta_c} n_k \frac{\partial \phi}{\partial x_k} \quad (12)$$

where this quantity is passively controlled by the fluid physics and allows a Neumann condition on density, $\rho$. The error from these penalized boundary condition converges as $O(\eta_c, \eta_b^{0.5})$.

3. Numerical Approach

In order to perform a particle-resolved direct numerical simulation of shock-particle interaction, high resolution is required to fully resolve the flow features around the particles and shock waves. However, high resolution is not required uniformly throughout the domain. Thus, an adaptive grid framework based on the parallel adaptive wavelet collocation method (PAWCM) is used to perform the simulations. The PAWCM is based on second-generation wavelets [40]–[43] and determines the grid points necessary to represent a solution based on a prescribed error threshold parameter $\epsilon$ and maximum level of resolution $j$. This allows a solution to be represented with a prescribed level of accuracy on much fewer grid points than what is traditionally necessary.

The hyperbolic solver developed for the PAWCM [44] is used to capture the wave structures and maintain numerical stability. This method is first order accurate near discontinuities such as shock waves and has higher accuracy in continuous regions. The spatial discretization in the continuous regions uses fourth-order finite-differencing and the time integration is based on the Crank-Nicolson method.
3.1 Averaging Method

To quantify flow unsteadiness and understand the significance of velocity fluctuations, mean flow statistics must be calculated. The phase average quantities of the gas phase, $\langle Q \rangle$ are obtained using

$$\langle Q \rangle = \frac{1}{V} \int_V Q dV$$

where $V$ is the sampling volume in the gas phase. In the 2D simulations performed in this work, the sampling volume becomes a sampling area. The sampling area ($V$) is as thin as 3 cells in the $x$-direction and spans the entire domain height in the $y$-direction. This equation is used to obtain the mean pressure and density at each $x$-position. The Favre average of a quantity $Q$ is defined as

$$\tilde{Q} = \frac{\int_V \rho Q dV}{\int_V \rho dV} = \frac{\langle \rho Q \rangle}{\langle \rho \rangle}$$

3.2 Validation and drag force

The evolution of the unsteady drag coefficient during the early interaction of a shock wave with a single particle is studied to replicate the experiment of Abe et al. [45] and validate the flow solver. In this interaction, the shock Mach number, $M$, has a magnitude of 1.7 and is defined as the ratio of the slip velocity to the local speed of sound. The particle Reynolds number based on the particle diameter, $D$ is considered to be $2.5 \times 10^5$ and is defined as

$$Re_p = \frac{\rho_s u_s D}{\mu_s}$$

The particle Reynolds number is proportional to the acoustic Reynolds number for the non-dimensional governing equations, Eq.(9) to (11) by,

$$Re_a = Re_p \left( \frac{\rho_0}{\rho_s} \right) \left( \frac{1}{M} \right) \left( \frac{\mu_0}{\mu_s} \right).$$
where subscript $s$ denotes the post-shock condition.

The jump condition is defined using

$$Q = Q_s - 0.5(Q_s - Q_0) \left[ 1 + \tanh \left( \frac{x_i - x_{i0}}{\delta} \right) \right]$$

(17)

where $Q = \{ \rho, u, T \}$ is the vector of primitive variables with $\rho$ being the density, $u$ the velocity, and $T$ the temperature. The post-shock conditions $Q_s = \{2.20, 0.93, 1.46\}$ and pre-shock conditions $Q_0 = \{1, 0, 1\}$ are prescribed using Rankine–Hugoniot jump conditions. The simulation is performed for a particle located at the origin with non-dimensional diameter, $D = 1$, in a rectangular computational domain of $(X \times Y) = [-L, L] \times [-0.5L, 0.5L]$, where $L/D = 11.4$. The initial shock location is $x_{i0} = -0.52D$ and the jump transition distance is $\delta = 10^{-4} D$. The undisturbed air downstream of the planar shock is initially at rest ($u_0 = 0$). The post-shock condition is prescribed at the inlet and non-reflecting boundary conditions are imposed on other faces.

The unsteady drag coefficient is calculated using

$$C_D = \frac{\vec{F} \cdot \hat{e}_i}{0.5 \rho_s u_s^2 A}$$

(18)

where $\vec{F}$ is the force acting on the particle and $\hat{e}_i$ is the unit vector in the streamwise direction, $\rho_s$ is the post-shock density, $u_s$ is the corresponding post-shock velocity and $A$ is the cross-section of the particle, which is equal to the particle diameter in the 2D simulation [46], [47]. The force components are obtained using the integral over the outer surface of the particle ($\delta \Omega$)

$$F_i = \int_{\delta \Omega} f_i dS$$

(19)

where $f_i = \sigma_{ij} n_j$ is the force acting on a differential surface $dS$, $n_j$ is the outward pointing normal and $\sigma_{ij} = -p \delta_{ij} + \tau_{ij}$ is the total stress tensor. The surface integral is changed to a volume
Using the divergence theorem, the integral can be approximated on a discrete grid by summing over all grid points \( k \) inside the particle of volume \( \Omega \),

\[
F_i = \iiint_{\Omega} \frac{\partial \sigma_{ij}}{\partial x_j} dV \approx \sum_{k \in \Omega} \left( \frac{\partial \sigma_{ij}}{\partial x_j} \right)_k \Delta V_k.
\]  (20)

Figure 1 compares the evolution of the unsteady drag coefficient over the particle obtained from the numerical solution, with the number of points per particle \( N_p = 176 \), against the experimental results reported by Abe et al. [45]. The unsteady drag coefficient experiences a maximum after being impacted by the shock. The magnitude of the maximum drag, which is 3.23, and the drag profile over time obtained from simulation are in good agreement with the experimental data. As expected, the drag during the early times shown in Figure 1 is dominated by pressure drag and contains very little if any contribution from viscous forces.

Since the time period of interest is from when the shock wave passes to when steady-conditions are formed, time is non-dimensionalized by the acoustic time of the particle \( \tau_d \),

\[
\tau_d = \frac{D}{c_0}
\]  (21)

which is the ratio of the particle diameter (\( D \)) over the speed of sound of the undisturbed gas, calculated as \( c_0 = \sqrt{\gamma p_0/\rho_0} \). Similar timescales such as the shock particle interaction time and inviscid timescales can be used, but are all of the same order [49]. The timescale associated with viscous forces is defined \( \tau_v = \delta_v^2/v_s \), where \( \delta_v/D \cong 1/\sqrt{Re_p} \) and \( Re_p \) is the particle Reynolds number based on the post-shock velocity. This timescale can be rewritten in terms of the acoustic timescale \( \tau_d \) so that \( \tau_v \equiv c_0/u_s = \tau_d/M_{ps} \), where \( M_{ps} \) is the Mach number of the post-shock flow relative to the particles. This suggests that the timescale associated with viscous forces is on the same order as the acoustic timescale. This is the same conclusion reached by Mehta et. al. [49] (note that they conclude that the viscous time is approximately twice as large as the shock passage.
time over a particle, which is consistent with our finding based on the acoustic time scale for particle transit; also they use the kinematic viscosity of the medium in the definition of the viscous time scale whereas we use the post-shock kinematic viscosity \( \nu_s \). This scaling is consistent with the observation that the Euler and NS solutions closely follow each other for times which are small with respect to the viscous time scale, with discrepancies showing up after a couple of acoustic transit time for a particle. The ratio of the particle motion time scale to the acoustic time scale based on the second law with the force given by Stokes drag is \( \tau_p / \tau_d = (\rho_p / \rho_s ) (Re_p/18) (c_0/u_s) \). With the density ratio \( \rho_p / \rho_s = O(10^3) \), \( Re = O(10^5) \) and \( c_0/u_s = O(1) \), \( \tau_p / \tau_d = O(10^7) \), which means the particles do not move appreciably over the course of the simulation [46], [49].

![Figure 1](image)

**Figure 1.** Comparison of the unsteady drag force obtained from the numerical results with the experimental data of Abe et al. [45]

4. **Shock impacting a transverse array of particles**

Although the primary focus of this paper is on the shock-particle cloud interaction, in this section we start with the investigation of shock interaction with a transverse array of particles to simplify the problem and provide a backdrop for understanding the more complex behavior of a
shock wave moving through a particle cloud. This simplified problem reveals the formation of complex wave structures that originate from neighboring particles. Mehta et. al. [46] performed a similar investigation via a two dimensional simulation based on Euler equations. Simulations using the Navier-Stokes equations can reveal the wave-wake interactions between the complex wave systems and the wake behind each particle, the evolution of local supersonic zones (LSZs), defined by Xu et. al [50], over the wake of each particle and the onset of unsteadiness under these interactions.

To simulate the shock interaction with a transverse array of particles, we consider the particle array as periodic images of a unit cell consisting of one particle with non-dimensional diameter $D = 1$, in a computational domain of $(X \times Y) = [-1.5L, L] \times [-0.5L, 0.5L]$, with $L/D = 11.4$ and impose periodic boundary conditions in the transverse direction. The particle diameter is considered to be the characteristic length scale. The transverse particle spacing between adjacent particles is $L$. In order to remain consistent with Regele et al. [31] and Wagner et al. (2012), a shock Mach number of 1.67 and a particle Reynolds number based on the particle diameter, $D$ of 3100 is used. The Rankine-Hugoniot jump condition of the shock is defined using the tangent hyperbolic function in Eq. (17) with the post-shock conditions $Q_s = \{\rho, u, T\}_s = \{2.14, 0.89, 1.44\}$ and pre-shock conditions $Q_0 = \{\rho, u, T\}_0 = \{1, 0, 1\}$. The shock wave is initially located at a non-dimensional axial location $x_{i0} = -0.52D$ and the particle is located at the origin. The undisturbed air downstream of the planar shock is initially at rest ($u_0 = 0$). For this problem, the post-shock condition is prescribed at the inlet ($x_{in} = -1.5L$) and a non-reflecting boundary condition [51] is imposed as the outlet condition (at $x_{in} = L$). Similar to the validation case, time is non-dimensionalized by the acoustic time of the particle $\tau_d$ defined in Eq. (21).
Figure 2 depicts the initial evolution of the wave system around the particle in a unit cell at two non-dimensional times $t = 0.83$ and $t = 2.77$. The top half contains numerical Schlieren images using the density gradient and the bottom half is colored by the flow Mach number. Similar to other works [36], [52]–[56], we first observe the formation of an upper shock wave system consisting of the incident shock ($IS$), the reflected shock ($R_1$), the slip surface ($S_1$), and the Mach stem ($M_1$) at the early time of interaction in Figure 2a. Then, as illustrated in Figure 2b, when the shock propagates further downstream the Mach stem is reflected at the plane of symmetry and the lower shock-wave system is formed. This consists of the Mach stem of the upper system ($M_1$), a second reflected shock wave ($R_2$), a second slip surface ($S_2$), and a second Mach stem ($M_2$). Figure 2 also shows that a local supersonic zone (LSZ), presented by sonic contour lines ($M = 1$), forms on the particle due to flow acceleration and grow over the boundary layer and wake behind the particle.

![Figure 2. Initial evolution of the wave system around each particle at $t = 0.83$ and $t = 2.77$. Top: The numerical Schlieren image. Bottom: Mach number contour. Local supersonic zones, represented with sonic lines, are shown on top and bottom of the particle.](image)
Figure 3. Wave-wave and wave-wake interaction between the neighbouring particles in two adjacent cells presented by the time series of Schlieren image at a) $t = 5.04$, b) $t = 7.32$, c) $t = 9.60$, d) $t = 15.30$, e) $t = 22.14$, f) $t = 25.56$. The red curves represent the LSZs. Particle diameter is $D$ and the particle spacing between the adjacent particles is $L = 11.4D$. 
As the incident shock propagates downstream, the wave system of the particle grows toward the cell boundary and starts to interact with the wave system of the neighboring particles in the adjacent cell in the transverse direction. Figure 3 shows the time evolution using numerical Schlieren images of the two neighboring particles in the adjacent cells. The wave-wave interaction, which is the mutual interaction between the wave systems of the two neighboring particles, is shown in Figure 3a. In Figure 3b the incident shock (IS) and Mach stems \((M_1)\) and \((M_2)\) of both particles superimpose to form the transmitted shock \((TS)\). As shown in Figure 3c, the wave-wake interaction starts once the reflected shocks reach the wake behind the particles. Some portion of the reflected shock \((R_{1,2})\) travels upstream of the wake and superimposes with the reflected shocks upstream of the particle and eventually form a cumulative reflected shock \((RS)\) upstream of the particle Figure 3d. The other portion of the reflected shock \((R_{1,2})\) along with \(R_2\) continues to reverberate downstream of the particle while interacting with the wake. The asymmetry and the waves appearing in the wake in Figure 3d suggests the commencement of Kelvin-Helmholtz instability from this interaction. This instability leads to unsteadiness and asymmetric vortex shedding under the effect of continuous wave-wake interactions in Figure 3e-f.

The LSZs grow throughout the wake during this interaction and induce stretching effects on the wake behind the particle (Figure 3 a-d). Figure 3e shows the LSZs of the neighboring particles merge together and a shock forms between the wakes of neighboring particles, which indicates the flow is choked due to the convergent-divergent geometry formed by the particles and the wakes behind them. The shock location in the wake dictates the location of vortex roll-up. The formation of the LSZs on the vortices increases the size of eddies and contributes to the formation of large structures (Figure 3e-f).
To test the grid dependence of the solution, this problem is tested over three different resolutions based on the effective number of grid points per particle diameter, namely $N_p = 44$, 88, and 176. Figure 4 compares the evolution of the unsteady drag coefficient for the three resolutions. For all three cases the drag coefficient increases until it reaches a maximum value of 3.5. Note that this maximum value is slightly larger than what is observed in Figure 1 because the Mach number and Reynolds number for this case are smaller than the former. This is consistent with the literature[8], [46], [49], [55], [57] where the unsteady drag coefficient is a function of both the Reynolds number and the Mach number and increases if either of these nondimensional numbers decreases. Figure 4 shows that the unsteady drag decreases until $t = 10.4$. This time period corresponds to the time between Figures 3c and d where the reflected shock from the neighboring particle reaches the surface of the particle. This time is called the non-dimensional acoustic-particle interaction time [46], which is defined as the time it takes for an acoustic wave (or shock wave) to travel from one particle to another and is given by $t_{ap} = (\Delta/D - 1)$. As mentioned earlier, $\Delta$ is the particle spacing and in this problem it is equal to 11.4 $D$, which gives $t_{ap} = 10.4$. It is worth mentioning that $t_{ap}$ is non-dimensionalized by acoustic time of the particle
(t_d), defined in Eq. (21). Excellent agreement exists for the unsteady drag coefficient until $t = 2t_{ap} = 22.8$ when the flow is dominated by gasdynamic processes with shock waves inducing flow and reflecting off of particles. During this time, the wake behind the particle is mostly symmetric but eventually destabilizes and asymmetry is introduced. At $t = 2t_{ap}$ the second wave from the neighboring particle approaches the surface of the particle and interacts with the wake and completes the onset of unsteady vortex shedding. As expected, some variability exists in the drag coefficient due to numerical diffusion. However, the results appear to be converging with increasing resolution and the difference between the $N_p = 88$ and 176 cases is small. This suggests that the impact of the grid dependence for the number of grids above $N_p = 88$ is minor. Mehta et al. [46], [49] also report that $N_p = 80$ appears to be sufficient resolution to resolve the flow behavior.

5. Particle cloud behavior

In this section the particle cloud is impacted by both shock and compression waves. The shock wave simulations demonstrate how flow unsteadiness originates within the cloud from both shock-induced and shear-related forces. The gradually-induced flow cases remove the shock-induced source of unsteadiness. Comparison of the two cases makes it possible to 1) verify that the initial shock induced flow unsteadiness eventually decays to the same flow unsteadiness level without a shock, 2) show that the shock induced unsteadiness is initially larger than the gradually-induced flow and 3) provide an estimate of how long the shock induced unsteadiness lasts.

The particle cloud configuration is based on the configuration proposed by Regele et. al [31], shown in Figure 5. The particle cloud thickness is used as the reference length and the particle diameter is found based on the desired volume fraction $\alpha_d = 0.15$ where
\[ D^2 = \frac{4aL^2}{N\pi} \]  

and \( N = 24 \) is the number of particles. The particles are distributed in the \( x \)-direction with equal spacing \( \delta_x = L/N \) so that each particle occupies a unique \( x \)-location, which minimizes the fluctuations in plane-integrated cross-section. Then the particle rows are shuffled from the inline distributed arrangement. Finally, each consecutive column of particles is shifted in the positive \( y \)-direction by approximately one particle diameter. This configuration minimizes the fluctuations in averaged variables and introduces the possibility for the oscillations to tend toward zero as the number of particles becomes large. See Ref. [31] for a more detailed discussion of the configuration.

In this study, we focus on the early interaction of shock and compression waves with the particle cloud, thus based on Ref. [31] and [8] the particles are fixed in place. Ling et al. [8], Mehta et. al. [46] and Sridharan et. al. [58] justify this choice due to the ratio of velocity change in the particle to the fluid scaling with the fluid-to-particle density. Since the fluid-to-particle density
ratio is extremely small, the ratio of the changes in velocity is likewise small. For example, in the present case of glass particles in air [25], the density ratio is \( O(0.001) \) and thus the timescale associated with significant particle movement is long due to the large inertia of the particle. Therefore, it is reasonable to ignore particle movement in the time scale considered here.

The simulation is performed using the computational setup shown in Figure 6 for both the shock-induced (shock wave) and gradually-induced (compression wave) cases. The rectangular computational domain is \((X \times Y) = [-6L, 6L] \times [-0.5L, 0.5L]\) where \(L = 1\) is the thickness of the particle cloud, and \(L/D = 11.4\). The cloud is located at \(-0.5 \leq x \leq 0.5\). The shock and compression waves are initially located at \(x = -1.0\). The undisturbed air downstream of the waves is initially at rest, \(u_0 = 0\). A detailed discussion of the required grid resolution is contained in section 5.2. Similar to the particle array simulations, periodic boundary conditions are imposed in the transverse direction, the post-shock condition is prescribed at the inlet, and non-reflecting boundary conditions [51] are imposed at the outlet on the right. The post-shock conditions in the shock-induced case correspond to a \(M_s = 1.67\) shock wave.

![Figure 6. Initial pressure profile for a) shock-induced case, b) gradually-induced case.](image)

In the gradually-induced case, the two states are separated over a larger distance to create a compression wave. The compression wavelength is chosen to be long enough that the pressure
changes much more gradually as it passes through the cloud to minimize any flow unsteadiness associated with high frequency wave reflections. This is done by choosing $\delta$ in Eq. (17) to be equal to the particle cloud thickness $\delta = L$. By doing this, the timescale associated with establishing the flow conditions is much longer than the shock induced case and minimizes the amplitude of unsteady wave motion that may be generated within the cloud to establish steady flow conditions.

5.1 Evolution of the wave system and local supersonic zones

The evolution of the complex wave system in the particle cloud can be best described using the effect of flow dilatation. The dilatation is the divergence of velocity ($\nabla \cdot \vec{u}$), which is non-zero for compressible flow. This term appears in the non-conservative form of the continuity equation as a source term:

$$\frac{1}{\rho} \frac{D\rho}{Dt} = -\nabla \cdot \vec{u}$$

where a non-zero dilatation indicates that the density is changing. Figure 7 contains snapshots of dilatation ($\nabla \cdot \vec{u}$) at several different instances after the shock first encounters the particle cloud. In these figures and all the following numerical results, time is non-dimensionalized by the acoustic time of the cloud $\tau = L/c_0$. Negative dilatation (shown in black) represents flow compression while positive values (shown in white) represent flow expansion.

Figure 7a shows that when the incident shock first hits the particle cloud, a collective reflected bow shock is created ahead of the cloud, which is comprised of multiple shock reflections, one from the wave system of each particle. A collective transmitted shock is also formed downstream due to the superposition of the incident shock and the Mach stems of all neighboring particles. Expansion fans form on each particle, which introduces non-zero dilatation. Figure 7b shows that, as time proceeds, the transmitted shock impinges on the later particles and additional reflected
waves from those particles interact with the wave systems of the leading particles and increase the complexity of the wave system. Portions of these waves propagate upstream and increase the amplitude of the cumulative reflected shock. The white areas in the figure indicate positive dilatation, which shows that expansion waves are induced at some point in time near each particle.

![Figure 7. Snapshots of the dilatation contours after the interaction of shock with the particle cloud at a) $t = 0.43$, b) 0.56, c) 1.00, d) 2.10, e) 3.2.](image)

As the transmitted shock emerges from the cloud (Figure 7c), the reflected shock waves start to dissipate near the leading edge of the cloud. The flow expansion along these particles also reduces (Figure 7c-e) and propagates into the cloud as time proceeds. However, the shock waves and expansion waves continue to persist at the trailing positions of the cloud. The persistence of these waves is due to the convergent-divergent flow geometry created by the presence of the particles that creates a choked flow point at the trailing edge of the cloud. Thus, as the gas emerges from the cloud it accelerates to supersonic speed. This creates an $O(1)$ density variation that
corresponds to a large dilatation in the cloud and wake region. Figure 7d-e indicates the presence of weaker shocks reverberating downstream of the cloud.

It should be noted that the strength of the shock wave diminishes as it passes through the cloud. The incident pressure and velocity decrease by 34% and 49%, respectively.

![Figure 8](image)

Figure 8. The evolution of local supersonic zones (LSZ) in the snapshots of the Mach numbers contours after the interaction of shock with the particle cloud at a) \( t = 0.43 \), b) 0.56, c) 1.00, d) 2.10, e) 3.2.

Snapshots of the instantaneous flow Mach number contour are depicted in Figure 8. As the shock propagates through the cloud the flow accelerates over each particle. Local Supersonic Zones (LSZs) appear over the particles (Figure 8a) and grow (Figure 8a-b) due to the mutual wave-wave interaction between the neighboring particles and eventually leads to choked flow conditions. Figure 8c-e shows that as the transmitted shock leaves the particle cloud, the LSZs travel downstream and accumulate mostly around the choked points at the leading edge of the cloud and
the wake behind. This provides evidence of the acceleration of the flow to supersonic speeds while leaving the cloud.

5.2 Grid convergence

In Section 4 it was found that using \( N_p = 176 \) cells across a particle diameter was sufficient to minimize the grid sensitivity of the unsteady drag coefficient. In this section the same resolution is used, but it is prudent to analyze the sensitivity of the mean and fluctuating flow fields since these are primary quantities of interest. Thus, in this section a grid sensitivity study is performed for both the mean streamwise velocity (\( \bar{u} \)) and the fluctuating velocities. The same resolution used in Section 4 is used with \( N_p = 44, 88, 176 \).

The fluctuation in the fluid velocity field (\( u'' \)) are defined with respect to the Favre averaged fluid velocity (\( \bar{u} \)) as \( u'' = u - \bar{u} \). The Root Mean Squared (RMS) of the velocity fluctuations is defined

\[
u_{rms} = \sqrt{u''^2} = \sqrt{u^2 - \bar{u}^2} \tag{24}\]

Figure 9a-c demonstrates the mean streamwise velocity \( \bar{u} \), and RMS velocities in streamwise (\( u_{rms} \)) and transverse (\( v_{rms} \)) directions as a function of position in streamwise direction, \( x \), for the three resolutions, at non-dimensional time \( t = 3.2 \). In these figures, the particle cloud is located between \(-0.5 < x < 0.5\) and the wake behind the cloud is located between \(0.5 < x < 2.5\). For all three resolutions, the mean velocity (Figure 9a) demonstrates convergence, however with the fluctuating velocities (Figure 9b-c) there are still some variations between the magnitude and phases at some locations. These variations occur near the trailing edge of the cloud because of numerical viscosity present in both shock waves and the shear layers in the wake region. Overall, the results for the \( N_p = 176 \) case suggests that this level of resolution is sufficient to capture the
reflected shock, transmitted shock, contact discontinuity as well as the mean flow field statistics and averaged magnitude of the velocity fluctuations. Thus, this resolution is used to represent the results for the particle cloud test cases.

Figure 9(b,d) show spikes in $u_{rms}$ at the locations of the reflected ($x = -2.2$) and transmitted ($x = 3.7$) shock locations. These spikes are numerical in nature because the shock is resolved over several points and the RMS velocity is poorly defined inside a shock wave.

![Graphs showing grid convergence study](image)

Figure 9. Grid convergence study for a) mean streamwise velocity, b) streamwise RMS velocity, c) transverse RMS velocity. d) Comparison of mean stream-wise velocity ($\bar{u}_1$) with the stream-wise, $u_{rms}$, and transverse, $v_{rms}$, velocity profile at $t = 3.2$.

A comparison of the mean flow field and RMS velocities is shown in Figure 9d at a non-dimensional time $t = 3.2$ to illustrate the relative importance of the fluctuating field to the mean
flow field. The stream-wise RMS velocity is larger than the transverse RMS velocity. Consistent
with earlier findings [31], the RMS velocities are the same order as the mean velocity, both inside
the cloud and in the wake region. However, as expected, the fluctuation amplitude is smaller in
the present work than what was observed in Euler simulations [31]. This is expected since
molecular viscosity is not present in the Euler equations, which may permit non-physical
oscillations. Use of the Navier-Stokes equation coupled with the IBM removes more of the noise
and non-physical oscillations associated with inviscid flow unsteadiness.

5.3 Analysis of the flow unsteadiness

The evolution of the unsteadiness is presented in Figure 10 using contour plots of the vorticity.
The instantaneous snapshots in this figure are taken at the same time as Figure 7 and Figure 8.
Therefore, the reader is referred to those figures for the corresponding wave-system and LSZ
locations.

Figure 10a-b shows that as the shock penetrates through the cloud, a boundary layer forms
around each particle. The boundary layers eventually separate under the effect of the local wave-
systems. The separated boundary layer (wake) behind each particle becomes unstable and vortex
shedding starts. The magnitude of vorticity inside the cloud increases between \( t = 1 \) and 2.1
(Figure 10c-d) as the number of the shocks and LSZs in the cloud increase, which indicates an
increase in unsteadiness during this period. Between \( t = 2.1 \) and 3.2 when the shock propagates
downstream, the magnitude of the vorticity decreases for the upstream particles whose positions
are \( x < 0 \) (Figure 10d-e), where the shocks have been dissipated and LSZs have moved
downstream. However, large unsteadiness is seen around the trailing edge of the cloud due to the
presence of shocks and choked flow conditions that persist in those areas and continuously interact
with the vortical structures. The vortical structures are elongated under the effects of LSZs. The
stretching effect is greatest on particles located at the trailing edge of the cloud where the flow is accelerating in larger LSZs and experiences larger expansion and dilatation, while leaving the cloud, which induces more stretching of the shear layers. Since the length of the vortices in the wake region is significantly longer than inside the cloud, it appears that the length of these structures in the cloud is limited by the presence of neighboring particles downstream.

Figure 10. Snapshots of the vorticity after the interaction of shock with the particle cloud at a) $t = 0.43$, b) 0.56, c) 1.00, d) 2.10, e) 3.2.

For deeper insight into the sources of unsteadiness in the shock-particle cloud interaction a budget analysis of the vorticity equation production terms is conducted. The evolution equation for vorticity in a compressible flow [59], [60] is written
\[
\frac{D\vec{\omega}}{Dt} = (\vec{\omega} \cdot \nabla)\vec{u} - \vec{\omega}(\nabla \cdot \vec{u}) + \frac{\nabla \rho \times \nabla p}{\rho^2} + \frac{1}{Re_a} \nabla \times \left( \frac{\nabla \cdot \tau}{\rho} \right)
\]

(25)

and describes the production and evolution of the fluid vorticity. In this equation, the left-hand side is the material derivative of the vorticity vector that describes the rate of change of vorticity. This change can be attributed to unsteadiness in the advection of vortices. The first term on the right-hand side represents the stretching or tilting of vorticity due to velocity gradients. This term is zero for the 2D analysis. The second term on the right-hand side is the vorticity-dilatation that describes stretching of vorticity due to flow compressibility. The third term on the right-hand side is the baroclinic term, which accounts for the production of vorticity due to misalignment of density and pressure gradients. The last term accounts for the diffusion of vorticity due to viscous diffusion. This term can be rewritten as

\[
\nabla \times \left( \frac{\nabla \cdot \tau}{\rho} \right) = \nabla \times \left( \frac{\nabla \cdot (\mu \nabla \vec{u})}{\rho} \right) = \nu \nabla \times \left( \nabla \cdot (\nabla \vec{u}) \right) = \nu \nabla \times \nabla^2 \vec{u} = \nu \nabla^2 \vec{\omega}
\]

(26)

assuming that the viscosity (\(\mu\)) is constant and \(\nu\) is the kinematic viscosity. This form describes the effect of viscous diffusion on the vorticity distribution. Analogues to the diffusion terms in the Navier-Stokes equations suggest that this term is always diffusive because the kinematic viscosity is always positive.

Figure 11 shows the dilatation, baroclinic, and diffusion source terms of the vorticity equation at a non-dimensional time of \(t = 3.2\) for the shock-particle cloud interaction case. Figure 11a shows the diffusion term that is present around the particles due to the shear induced by particles, and in the shear layers of vortical structures both inside the cloud and in the wake region. Due to the no-slip boundary condition at the particle surface, the viscous flow decelerates in a thin boundary layer along the surface, which produces vorticity. Subsequently, this vorticity is advected downstream with the fluid. Away from particle surfaces, this term diffuses vorticity.
Figure 11. Vorticity production at $t = 3.2$ for a) diffusion term, b) baroclinic term, c) vorticity-dilatation terms.

It can be seen that the diffusion term is larger around the trailing edge particles than the leading-edge particles. This can be explained by comparing this plot with the Mach number contour plot at the corresponding time (Figure 8e). Mach number contours indicate that the flow is slower in most locations near the leading edge while the flow is significantly faster near the trailing edge. As a result, stronger shear stress is present in the flow around particles closer to the trailing edge.

Figure 11b illustrates the baroclinic term. This term generates vorticity from unequal acceleration as a result of misalignment between the pressure and density gradients. In this condition, the pressure force on a fluid element does not pass through its center of mass and the pressure exerts a torque on the fluid element to generate vorticity or intensify pre-existing vorticity.
Comparison of Figure 11b with the vorticity profile (Figure 10e) and wave structure (Figure 7e) indicates that this effect is present where shocks collocate with vortical structures and is more dominant wherever shocks are stronger. The wave structure in Figure 7e shows that at $t = 3.2$ stronger shocks are located within the second half of the cloud and within the wake region behind the cloud. As a result, the baroclinic term is more significant in those locations.

Figure 11c. shows the vorticity-dilatation term at $t = 3.2$. Comparison of this figure with the dilatation contours at the corresponding time (Figure 7e) indicates that the vorticity-dilatation term acts as a source for amplifying pre-existing vorticity in the region of negative dilatation (compression) and as a sink to attenuate vorticity in the region of positive dilatation (expansion). The absolute value of this term is observed to be large in supersonic regions (see Figure 8e), near the trailing edge of the cloud and in the wake region.

The qualitative discussion of the vorticity source terms above helps identify the effect of each term on the evolution of vorticity and unsteadiness and tie the effect with the local flow features, such as wave structure, LSZs and local dilatation. To better quantify these three terms and demonstrate the relative importance of them in the strong flow unsteadiness, we present a quantitative discussion based on the comparison of their phase-averaged magnitude. Similar quantification is performed for a gradually-induced case.

The averaging method used to quantify the flow unsteadiness is described in section 3.1. Since the resultant curves are still oscillatory due to the strong flow unsteadiness, a spline curve with the smoothing factor of $sp = 0.998$ is fitted to the data set to create a smooth graph.
Figure 12. The magnitude of the averaged **Diffusion** (--), **Baroclinic** (-) and **Vorticity-dilatation** (··) terms at four times, \( t = 0.56, 1.2, 2.1, 3.2 \) for both **Shock-induced** (o) and the **Gradually-induced** (without markers) flow over the cloud. The cloud is located within \(-0.5 < x < 0.5\). The legend is set based on the first letter of each case (S or G) and first letter of each term (D, B or V).

Figure 12 shows the magnitude of the averaged diffusion, baroclinic and vorticity-dilatation terms at four times, \( t = 0.56, 1, 2.1, 3.2 \), for both the shock-induced and gradually-induced cases. To focus on regions with flow unsteadiness the results are plotted from \( x = -0.5 \) to \( x = 2.5 \). For both cases, the vorticity-dilatation term is the most dominant term at all considered times. The baroclinic and diffusion terms are both almost an order of magnitude less than the vorticity-dilatation term. The magnitude of each term for the shock-induced case is much greater than the
gradually-induced case. The order of the difference between the two cases for each term at the early time of interaction is larger than at later times. This indicates that the impulsive nature of the shock produces additional unsteadiness in the flow.

Figure 12a shows that for early times in the gradually-induced case, the diffusion term and the baroclinic term are of the same order. In this case, the baroclinic effect is larger in the first half of the cloud while the diffusion term is larger in the second half. This occurs because the induced flow transitions from low speed to high speed conditions further into the particle cloud. The strength of the reflected shock is proportional to the free stream velocity. Thus, the reflected shocks in the first half that have experienced higher free stream velocities than the second half of the cloud are stronger, which leads to greater baroclinic vorticity production from those particles. In the shock-induced case, since the reflected shock waves reverberate around inside the cloud, the baroclinic term is almost an order larger than the diffusion term.

As flow accelerates in the cloud (Figure 12b) the shear on the particles increases and thus the vorticity production from the diffusion term increases as well. The baroclinic term grows due to the formation of reflected shocks and shocklets all over the cloud. The vorticity-dilatation term grows because the flow remains transonic within the cloud (Figure 7c).

After the transmitted shock leaves the cloud (Figure 12b) the shock waves dissipate, which causes the baroclinic term to reduce. Figure 12c indicates that the decay starts from the leading edge and penetrates the cloud with time. Dilatation also diminishes in the cloud (Figure 7d-e) due to this transition and causes the vorticity-dilatation term to reduce as well (Figure 12c-d). However due to the choked flow conditions, local supersonic zones and finite dilatation around the trailing edge, all source terms maintain a peak value for $0.3 < x < 0.5$ at late times (Figure 12d).
In the wake, all vorticity production sources become smaller. In this region the dilatation and baroclinic terms are still free to produce more vorticity from shock waves and localized supersonic zones. However, in the absence of particles the diffusion term dissipates the existing vorticity. Once the flow is choked and passes through standing shocks to equalize the pressure the flow remains subsonic. This ensures that the baroclinic term decreases further into the wake region (Figure 7d). Finally, once the flow is subsonic the vorticity amplifying effect of the dilation term diminishes, which results in a reduction of vorticity-dilatation term (Figure 7e).

5.4 Kinetic energy in the fluctuating motion

The importance of the fluctuating field and the effect of fluctuating velocity on the flow behavior can be best described using the Reynolds stress term in the mean flow momentum equation. The trace of the Reynolds stress term is the kinetic energy in the fluctuating field, which is defined

\[ K = \frac{1}{2} \frac{\langle \rho u'_i u'_{i'} \rangle}{\langle \rho \rangle} = \frac{u''_i u''_{i'}}{2}. \]  

The average kinetic energy, \( E_k \), in the gas phase

\[ E_k = \frac{1}{2} \frac{\langle \rho u_i u_i \rangle}{\langle \rho \rangle} = \frac{\bar{u}_i \bar{u}_i}{2} \]  

is the sum of the kinetic energy in the mean fluid field, \( \bar{E}_k \),

\[ \bar{E}_k = \frac{\bar{u}_i \bar{u}_i}{2} \]  

and the average kinetic energy in the fluctuating field, \( \bar{K} \). It should be noted that the objective of the present work is to provide a better understanding of how flow unsteadiness is created in these situations and not to quantitatively predict the flow unsteadiness. The particle configuration developed by Regele et al. [31] provides a way to minimize fluctuations in the volume fraction
when calculating averaged quantities. Quantitative prediction must be performed with spherical particles in three dimensions using multiple particle arrangements.

Figure 13 shows a x-t diagram of the non-dimensional kinetic energy in the fluctuating field, $K$, for both the shock-induced and gradually-induced cases up to $t = 4$. For $t > 4$, changes in $K$ are minimal and the production of $K$ from viscous forces has reached steady state. It is evident that the average kinetic energy in the fluctuating field $K$ is present in both the cloud ($-0.5 < x < 0.5$) and the wake region (between $x = 0.5$ and the contact line) for both cases. In both cases the magnitude of $K$ is significant during the early phases of interaction. Comparison of the shock-induced case, Figure 13a, with the gradually-induced case, Figure 13b, shows that before about $t = 2.1$, when the flow is in the unsteady mode, the shock-induced case presents a higher magnitude of the kinetic energy in the fluctuating motion both inside the cloud and near the trailing edge of the cloud and it experiences a more rapid change in comparison to the gradually-induced case. In both cases, after $t = 2.2$ the flow becomes more steady, a decay in $K$ is observed due to the dissipation of shocks and compression waves and a reduction of wave-wake interactions. However, it is seen that $K$ holds a significant value at locations around the trailing edge of the cloud ($x \sim 0.5$) and the immediate wake region.
In Figure 14, the evolution of the kinetic energy over time in three specific locations of the particle cloud (where $x$ is $-0.3$, $0.0$ and $0.3$) is compared with that of the gradually-induced case to better illustrate the significance of the impulsive nature of shock waves on this evolution. At each location, the evolution of the kinetic energy in the fluctuating field, $K$, reaches a peak followed by decay over time and oscillates around some mean value for both cases. The peak value for the shock-induced case is larger at all locations. The difference between the peak values is indicative of the impulsive effect of shocks on the appearance of the fluctuating field at those locations. This effect is more dominant in the particles closer to the leading edge, $x = -0.3$ and it decreases as we reach $x = 0.3$. At each location the peak occurs at a later time for the gradually-induced case due to the delay of impact over the large transition distance, $\delta$, for the compression wave.
Figure 14. Comparison of kinetic energy in the fluctuating motion at three different positions, $x = -0.3, 0.0, 0.3$, of the particle cloud for the shock induced (S) and gradually-induced cases (G).

As expected, Figure 14 shows that the mean values of $K$ for the shock and gradually-induced cases converge as the flow begins to steady. The magnitude of the steady-state value of $K$ is larger near the trailing edge of the cloud where transonic flow conditions and shock waves exist because of choked flow conditions. This leads to continuous wave-wake interaction between these shock waves and the expanded vortical structures that introduce continuous instability and enhances velocity fluctuations [50], [61], [62].

Comparison of the kinetic energy in the fluctuating field, $K$, with the kinetic energy in the mean flow field, $\overline{K}$, reveals the importance of the fluctuating field generated under the effect of the shock on the particle cloud. This comparison is demonstrated in Figure 15 at four different non-dimensional times, $t = 0.56, t = 1, t = 2.1$ and $t = 3.2$. At $t = 0.56$ (Figure 15a). When the transmitted shock is inside the cloud, the kinetic energy in the fluctuating field, $K$, is developing and reaching the kinetic energy in the mean flow field $\overline{K}$. 
Figure 15. Comparison of the mean kinetic energy with the kinetic energy in the fluctuating field at a) $t = 0.56$, b) $t = 1$ c) $t = 2.1$ d) $t = 3.2$.

Figure 15b shows that, as the transmitted shock emerges from the cloud at $t = 1$, $K$ has increased all over the cloud while $\overline{E_k}$ has decreased. This means that the energy has been transferred from the mean flow field to the fluctuating field. This leads to $K$ having a larger value than $\overline{E_k}$ in almost 60% of the cloud. This occurs from multiple reflected shocks that continuously interact with the highly unsteady wake and enhances the kinetic energy in the fluctuating motion.

As the transmitted shock travels downstream (Figure 15c-d) both $K$ and $\overline{E_k}$ decrease in the leading locations of the cloud because the flow regime has changed to subsonic in these regions and the shock waves have dissipated (see Figure 7 Figure 8). However, towards the trailing edge
they still hold larger values because of the persistence of the shock waves and LSZs in those areas. The ratio of $K/E_k$ is approximately one both inside the cloud and in the wake region.

These results show that shock waves induce a significant amount of kinetic energy in the fluctuating motion during the early times. Comparison of the magnitude of kinetic energy in the fluctuating motion and the kinetic energy in the mean flow field shows that $K$ contributes significantly to the average kinetic energy, $E_k$. Since $K$ is the trace of the Reynolds stress term it implies that this term in the momentum equation and the corresponding unclosed terms in the energy equation cannot be neglected while attempting to model shock-particle cloud interaction in the dense regime.

Additional simulations, not included here, were performed to examine the sensitivity of the results to the compression wave thickness. As the thickness increases the maximum in $K$ decreases, moreso in the front half of the cloud than the back (see Figure 14). Presumably in the limit that the thickness is orders of magnitude larger than the cloud thickness there would be no maximum at all. We chose $\delta$ to be equal to the particle cloud thickness so that the high frequencies were filtered out, but there was still a distinguishable wave to compare with the shock driven case. The primary conclusion that the initial unsteadiness originates from the shock wave reflections where high frequencies may exist rather than viscous forces is not dependent on the thickness chosen.

### 5.5 Comparison with previous Euler simulations

In the previous Euler simulations [31] the RMS fluctuation velocities in the flow and transverse directions were shown to be on the order of the mean flow velocity. Figure 16a displays these results at a non-dimensional time $t = 2.7$. In Figure 16b, the mean and fluctuation velocities are plotted for the Navier-Stokes solutions at the same time. Note that while the mean flow
velocities are consistent between the two cases, the RMS velocities in the NS solutions are about 40% lower than the Euler solution. This is anticipated because the additional viscous forces damp the fluctuating motion and thereby give a smaller fluctuation amplitude. Nevertheless, the RMS velocity is still on the order of the mean flow velocity, which is quite significant under these transonic flow conditions.

The kinetic energy in the fluctuating field, $K$, obtained from both the Euler and NS simulations are also compared in Figure 17. This comparison shows that $K$ both in the cloud ($-0.5 < x < 0.5$) and in the following wake region ($x > 0.5$) is less in the Navier-Stokes simulation. Again, this can be attributed to the viscous dissipation present in the viscous simulation, which dissipates the kinetic energy.
Figure 17. Comparison of the kinetic energy in the fluctuating field obtained from Euler and Navier-Stokes simulation at $t = 2.7$.

6. Conclusions

In this work the interaction of a shock wave with two different configurations of particles in the dense gas-solid regime, namely a transverse array of particles and a particle cloud is investigated. Particle-resolved direct numerical simulations are performed by solving the compressible Navier-Stokes equations coupled with an volume penalization method.

Simulations of a shock interaction with a transverse array of particles reveals the evolution of the wave system, local supersonic zones, and the wake behind each particle as well as the commencement of Kelvin-Helmholtz instabilities and vortex shedding under the effect of the wave-wave and wave-wake interactions between the neighboring particles. It is demonstrated that the unsteady drag coefficient of a cylinder after shock passage agrees well with experimental data. It is also shown that the drag coefficient and mean and unsteady flow velocities are relatively insensitive to grid resolution.

Shock interaction with a particle cloud in comparison with gradually-induced flow over the same particle cloud is investigated to quantify the flow unsteadiness and velocity fluctuations that
arise from these interactions. The sources of flow unsteadiness and vorticity generation are quantified by analyzing the vorticity production terms for compressible flows. It is shown that a primary source of vorticity comes from the viscous diffusion term when the no slip condition at particle surfaces creates strong shear forces. This vorticity is then advected downstream. The baroclinic term, which is larger than the diffusion term in most locations, generates vorticity where reflected shocks collocate with the vortical structures. The vorticity-dilatation term is almost an order of magnitude larger than the other two terms. It amplifies pre-existing vorticity in the region of negative dilatation and attenuates vorticity in the region of positive dilatation. The magnitude of each term for the shock-induced case is much larger than the gradually-induced case because of a shock waves natural ability to induce flow unsteadiness. The order of this difference reduces over time until the shock and gradually-induced cases reach the same unsteadiness levels.

To perform a detailed analysis of the importance of velocity fluctuations and kinetic energy in the fluctuating field, arising from the strong unsteadiness, phasic-Favre average statistics are calculated. Based on this analysis, the kinetic energy in the fluctuating field is the same order of magnitude as the kinetic energy in the mean flow field and contributes significantly to the mean kinetic energy. Thus, the Reynolds stress term in the momentum equation and the corresponding unclosed terms in the energy equation cannot be neglected while modeling the dense compressible flow regime. While this effect is true in general it is greater in shock-induced situations.

Logical next steps in this work include additional 2D studies of how the flow changes with varying Mach numbers, particle cloud volume fraction, temperature and heat flux in the fluctuating field, and then ultimately all of this performed in three dimensions. Approved for public release: LA-UR-17-26555.
References


[29] F. M. Najjar, J. P. Ferry, A. Haselbacher, and S. Balachandar, “Simulations of Solid-


119, no. 10, pp. 0–13, 2016.


1998.


