On progressive blast envelope evolution of charged particles in electromagnetic fields

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Highlights

• We investigate the explosion of a set of charged particles in an electromagnetic field and the progressive time evolution of the blast envelope.
• It is shown that the initial spherical blast envelope evolves into the shape of an ellipsoid whose longitudinal axis is aligned with the magnetic field. Specifically, the individual particles rotate around the longitudinal axis, and rotate in decaying orbits until they become stationary, leaving a stationary overall ellipsoidal configuration of particles.
• A direct multiparticle model is constructed, which balances the detonation energy released from the initial blast pulse with the subsequent particle-system kinetic energy and then computes the trajectories of the discrete interacting material under the influence of the electromagnetic field and drag from any surrounding medium.
• Under certain simplifying assumptions, the model can be solved for analytically, which provides a guide to identifying the key parameters that control the evolving blast envelope.
• Three dimensional examples are provided to illustrate the framework/method.

Abstract

In this paper, we investigate the explosion of a set of charged particles in an electromagnetic field and the progressive time-evolution of the blast envelope. It is shown that the initial spherical blast envelope evolves into the shape of an ellipsoid whose longitudinal axis is aligned with the magnetic field. Specifically, the individual particles rotate around the longitudinal axis, and rotate in decaying orbits until they become stationary, leaving a stationary overall ellipsoidal configuration of particles. In order to investigate this system, a direct multiparticle model is constructed, which balances the detonation energy released from the initial blast pulse with the subsequent particle-system kinetic energy and then computes the trajectories of the discrete interacting material under the influence of the electromagnetic field and drag from any surrounding medium. Under certain simplifying assumptions, the model can be solved for analytically, which provides a guide to identifying the key parameters that control the evolving blast envelope. Three dimensional examples are provided to illustrate the framework/method.

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1. Introduction

Routine analyses of blasts rarely address the scenario of a discharged system of charged particles in an electromagnetic field. However, there are a variety of areas in which a blast of charged particles can encounter an electromagnetic field, for example in the ionosphere, in astrophysical events associated with planet, solar-system and galaxy formation, the study of sprays, aerosol, plasmas and charged particle manipulation in manufacturing. For example, one application in particular, Coronal Mass Ejections (CMEs), is highly relevant to protection of the satellite and electronic infrastructure that now blankets the earth. Specifically, a CME is a blast of charged particles in the presence of the sun’s magnetic field. During active solar periods, the sun exhibits approximately three CMEs per day usually occurring where there are large clusters of sun spots. The ejected plasma of electrons and protons, which is essentially a shock wave, can cause a geomagnetic storm that propagates towards Earth, leading to potentially damaging effects on the aforementioned satellite and electronic infrastructure. This is also the source of the Aurora Borealis and also increased risk to humans at high altitudes. For more details see articles in the scientific and popular press: Christian [1], Fox [2], Gopalswamy [3], Baker et al. [4], Morring [5], Wilson et al. [6], Carrol and Ostlie [7], Andrews [8], Vourlidas et al. [9] and Manchester et al. [10].

In this paper, we investigate the explosion of a cloud of charged particles in an electromagnetic field and the progressive time-evolution of a blast envelope. It is shown that the initial spherical blast envelope evolves into shape of an ellipsoid whose longitudinal axis is aligned with the magnetic field. In the absence of an electromagnetic field the blast envelope would be spherical. The individual particles rotate around the longitudinal axis, which is aligned with the magnetic field. In the presence of drag, the individual particles rotate in decaying orbits until they become stationary, leaving a stationary overall ellipsoidal configuration of particles. In order to investigate this system, a model is constructed which balances the detonation energy released from the initial blast pulse with the subsequent particle-system kinetic energy and then computes the trajectories of the particles under the influence of the electromagnetic field and drag from any surrounding medium. Under certain simplifying non-interacting particle assumptions, the model can be solved for analytically, which provides a guide to identifying the key parameters that control the evolving blast envelope. Thereafter, a direct interacting multiparticle model and solution algorithm is constructed, and key features of the blast envelope with particle interaction are discussed. Three dimensional examples are provided to illustrate the framework/method.

2. Electromagnetically driven dynamics of a charged particle

We recall the following important observations in conjunction with electromagnetic phenomena (Jackson [11]):

- If a point charge $q$ experiences a force $\Psi^e$, the electric field, $E^{ext}$, at the location of the charge is defined by $\Psi^e = qE^{ext}$.
- If the charge is moving, another force may arise, $\Psi^m$, which is proportional to its velocity $v$. This other (induced) field is denoted as the “magnetic induction” or just the “magnetic field”, $B^{ext}$, such that $\Psi^m = qv \times B^{ext}$.
- If the forces occur concurrently (the charge is moving through the region possessing both electric and magnetic fields), then the electromagnetic force is $\Psi^{e+m} = qE^{ext} + qv \times B^{ext}$.

Remark. If we make the simplifying assumption that the electric field is externally-controlled $E^{ext} = (E_1^{ext}, E_2^{ext}, E_3^{ext})$, not dependent on the charged particles and that the magnetic field is also externally-controlled, $B^{ext} = (B_1^{ext}, B_2^{ext}, B_3^{ext})$, for single particles, the equations can be solved analytically (for example, see Jackson [11]). We consider a few of these cases, for static (“dead”) electromagnetic fields (Fig. 1), further assuming that the electric and magnetic fields are independent of one another.

2.1. Governing equations

We consider an isolated charged mass with position vector denoted by $r$, governed by $(\ddot{r} = v, \dot{r} = \dot{v})$

$$m\dot{v} = q(E^{ext} + v \times B^{ext}).$$

(2.1)

The governing Eq. (2.1), written in component form is, for component 1

$$\dot{v}_1 = \frac{q}{m}(E_1^{ext} + (v_2B_3^{ext} - v_3B_2^{ext})).$$

(2.2)
Fig. 1. An isolated particle makes circular orbits in a plane perpendicular to the static magnetic field. When $E_{3}^{\text{ext}} = 0$, this traces out the equation of a circle centered at $(0, -\frac{v_{o}w}{m})$. The radius of the “magnetically-induced circle” in the cyclotron radius.

for component 2

$$
\dot{v}_2 = \frac{q}{m} (E_{2}^{\text{ext}} - (v_1 B_{3}^{\text{ext}} - v_3 B_{1}^{\text{ext}})),
$$

(2.3)

and for component 3

$$
\dot{v}_3 = \frac{q}{m} (E_{3}^{\text{ext}} + (v_1 B_{2}^{\text{ext}} - v_2 B_{1}^{\text{ext}})).
$$

(2.4)

2.2. Qualitative features

Following Zohdi [12–17], we consider both the electric and magnetic fields to be present, $r(t = 0) = 0$, $v(t = 0) = v_o e_1$, $B_{3}^{\text{ext}} = B_{3}^{\text{ext}} e_3$ and $E_{3}^{\text{ext}} = E_{3}^{\text{ext}} e_3$, consequently, for a single particle

$$
\begin{bmatrix}
  v_1(t) \\
  v_2(t) \\
  v_3(t)
\end{bmatrix} = \begin{bmatrix}
  v_o \cos wt \\
  -v_o \sin wt \\
  \frac{q}{m} E_{3}^{\text{ext}} t
\end{bmatrix} \Rightarrow \begin{bmatrix}
  r_1(t) \\
  r_2(t) \\
  r_3(t)
\end{bmatrix} = \begin{bmatrix}
  \frac{v_o}{w} \sin wt \\
  \frac{v_o}{w} (\cos wt - 1) \\
  \frac{q}{2m} E_{3}^{\text{ext}} t^2
\end{bmatrix}
$$

(2.5)

where $\omega = \frac{q B_{3}^{\text{ext}}}{m}$ is known as the cyclotron frequency. The cyclotron frequency (gyrofrequency) is the angular frequency at which a charged particle makes circular orbits in a plane perpendicular to the static magnetic field. Notice that when $E_{3}^{\text{ext}} = 0$, this traces out the equation of a circle centered at $(0, -\frac{v_o w}{m})$. The radius of the “magnetically-induced circle” (radius of oscillation) is

$$
R \overset{\text{def}}{=} \frac{v_o}{\omega} = \frac{v_o m}{q B_{3}^{\text{ext}}}. 
$$

(2.6)

Thus, if a desired “turning radius” is denoted by $R$, one may solve for the magnetic field that delivers the desired effect, $B_{3}^{\text{ext}} = \frac{v_o m}{q R}$. We define the corresponding time period for one cycle to be completed as $T \overset{\text{def}}{=} \frac{2\pi}{\omega}$. The composite motion is that of a helix, since the third position component grows quadratically in time, while the other two components trace out a circle.

**Remark 1.** In the special case when there is no magnetic field, if $r(t = 0) = 0$, $v(t = 0) = v_o e_1$, $B_{3}^{\text{ext}} = 0$ and $E_{3}^{\text{ext}} = E_{3}^{\text{ext}} e_3$, the solution for the dynamics of an isolated particle is

$$
\begin{bmatrix}
  v_1(t) \\
  v_2(t) \\
  v_3(t)
\end{bmatrix} = \begin{bmatrix}
  v_o \\
  0 \\
  \frac{q}{m} E_{3}^{\text{ext}} t
\end{bmatrix} \Rightarrow \begin{bmatrix}
  r_1(t) \\
  r_2(t) \\
  r_3(t)
\end{bmatrix} = \begin{bmatrix}
  v_o t \\
  0 \\
  \frac{q}{2m} E_{3}^{\text{ext}} t^2
\end{bmatrix}.
$$

(2.7)

Thus, the third position component grows quadratically in time.
The progressive evolution of a blast envelope, where the longitudinal axis grows in the direction of the magnetic field. Generally: (a) the particles initially move radially-outward from the blast (b) the magnetic forces induce a rotational force in the $n \times B^\text{ext}$ direction, that starts a large-scale rotation about the $B^\text{ext}$-axis (c) the particles that were initially blasted in the direction of the $B^\text{ext}$-axis travel further in that direction (d) the drag forces slowly start to decay the energy of the particles, and the orbits become progressively smaller and (e) the drag forces eventually absorb all the energy, and the particles cease to move.

Remark 2. In the special case with no electric field and a magnetic field present, $r(t = 0) = 0, v(t = 0) = v_o e_1$, $B^\text{ext} = B^\text{ext}_3 e_3$ and $E^\text{ext} = 0$. Consequently, for a single particle, the solution is

\[
\begin{align*}
\begin{bmatrix} v_1(t) \\ v_2(t) \\ v_3(t) \end{bmatrix} &= \begin{bmatrix} v_o \cos \omega t \\ -v_o \sin \omega t \\ 0 \end{bmatrix} \Rightarrow \begin{bmatrix} r_1(t) \\ r_2(t) \\ r_3(t) \end{bmatrix} = \begin{bmatrix} \frac{v_o}{\omega} \sin \omega t \\ \frac{v_o}{\omega} (\cos \omega t - 1) \\ 0 \end{bmatrix}.
\end{align*}
\]

At steady state, for a particle traveling with velocity $v_{ss}$, the cyclotron radius can be derived by equating radially-outward forces to magnetic forces

\[
\frac{m v_{ss}^2}{R} = q v_{ss} \|B^\text{ext}\| \Rightarrow R = \frac{m v_{ss}}{q \|B^\text{ext}\|}.
\]

The time-period for one revolution is

\[
2\pi R = T v_{ss} \Rightarrow T = \frac{2\pi R}{v_{ss}} = \frac{2\pi m}{q \|B^\text{ext}\|},
\]

leading to the cyclotron frequency $T = \frac{2\pi}{\omega} \Rightarrow \omega = \frac{q \|B^\text{ext}\|}{m}$.

3. Specific blast-driven dynamics

We now qualitatively study the time-evolution of the envelope of a cloud emanating from a blast. The immediate objective is to first develop a simplified, qualitative, model whereby the particles do not interact with one another, and which captures the essential physics of detonation and blast envelope growth. Afterwards, a “brute-force”, full-interaction approach is developed and the results compared.

3.1. Assumptions

A schematic of the model problem is shown in Fig. 2. We make the following simplifying assumptions:

- The blast particles do not interact with one another.
The blast particles are all the same size, assumed spherical with radius \( R_i = R \) and receive the same velocity pulse (denoted \( \delta v(0) \)), in the radial direction from the center of the blast upon detonation. Specifically, the velocity vector pulse is radially outward from the center of the sphere, co-located at the center of mass of material:

\[
\delta v_i(0) = \|\delta v(0)\| \left( \frac{r_i(0) - r_c(0)}{\|r_i(0) - r_c(0)\|} \right) \overset{\text{def}}{=} \|\delta v(0)\| n_{ri}
\]

where \( r_i \) is the position vector of the \( i \)th particle, \( n_{ri} \) is the normal/radial direction and

\[
r_c(0) = \frac{1}{N} \sum_{i=1}^{N} m_i r_i(0),
\]

where \( N \) is the number of particles, \( r_c(0) \) is the center of mass of the packed particles and \( m_i \) is the mass of each particle. The pulse velocities are added to the velocity vectors immediately before the pulse (\( v^{-}(0) \))

\[
v_{i}^{+}(0) = v_{i}^{-}(0) + \delta v_{i}(0).
\]

The magnitude of the initial velocity pulse dictates initial energy released (\( W \)), which is assumed to be converted into kinetic energy for the blast material at (\( t = 0 \)):

\[
W = \sum_{i=1}^{N} \frac{1}{2} m_i \|\delta v(0)\|^2 \Rightarrow \|\delta v(0)\| = \sqrt{\frac{2W}{\sum_{i=1}^{N} m_i}},
\]

where \( \delta v(0) \) is the velocity of pulse imparted to a particle in the radial direction, \( M \) is the total blast material mass, \( m_i = \rho_i \frac{4}{3} \pi R_i^3 \) is mass of the individual particles, where \( \rho_i \) is the density of the particles.

- The objects in the system are assumed to be small enough to be considered (idealized) as particles, spherical in shape, and that the effects of their rotation with respect to their mass center are unimportant to their overall motion. The equation of motion for the \( i \)th particle in the system is

\[
m_i \ddot{v}_i = \Psi_i^{in} = \Psi_i^{drag} + \Psi_i^{e+m},
\]

with initial velocity \( v_i(0) \) and initial position \( r_i(0) \).

- For the drag, we will employ a general phenomenological model

\[
\Psi_i^{drag} = \frac{1}{2} \rho_a C_D \|v^f - v_i\| (v^f - v_i) A,
\]

where \( C_D \) is the drag coefficient, \( A \) is the reference area, which for a sphere is \( A = \pi R^2 \), \( \rho_a \) is the density of the ambient fluid environment and \( v^f \) is the velocity of the surrounding medium which, in the case of interest, is air.

Remark. We ignore gravity and buoyancy. For investigations of “classical”, non-electromagnetic blasts, see Zohdi [18]. Also, we will assume that \( v^f \approx 0 \), implicitly assuming that the dynamics of the surrounding medium is unimportant. However, for other applications, such as high-speed flow, the motion of the surrounding fluid can be important, necessitating fully coupled (two-way) particle–fluid interaction models. This is outside the scope of the present work. Generally, this requires the use of solid–fluid staggering-type schemes (for example, see Zohdi [12–17] and Avci and Wriggers [19]). This is discussed further at the end of the paper.

### 3.2. Purely electromagnetic effects

If the basic governing equation,

\[
m \ddot{v} = q(\mathbf{E}^{ext} + \mathbf{v} \times \mathbf{B}^{ext}) \overset{\text{def}}{=} \Psi^{e+m}
\]

is augmented with an initial condition of outward radial blasts, \( v(t = 0) = v_o \mathbf{n} \), and we ignore the Electric field, we have

\[
m \ddot{v}(t = 0) = q v_o (\mathbf{n} \times \mathbf{B}^{ext}).
\]
The cross product of $\mathbf{n} \times \mathbf{B}^{\text{ext}}$ yields a force that is always perpendicular to the $\mathbf{B}^{\text{ext}}$ field. For example, consider $\mathbf{B}^{\text{ext}} = \mathbf{B}^{\text{ext}}e_3$ and a particle that is initially projected in the $x_1$ direction. Initially, the $qve_1 \times be_3$ the force pushes the particle in the $-x_2$ direction. Subsequently, the $-qve_2 \times B^{ext}e_3$ the force pushes the particle in the $-x_1$ direction, then the $-qve_1 \times B^{ext}e_3$ the force pushes the particle in the $+x_2$ direction and the $qve_2 \times B^{ext}e_3$ the force pushes the particle in the $+x_1$ direction. The radius of this path is the Cyclotron radius. Furthermore, any particle, by virtue of the cross product of $\mathbf{n} \times \mathbf{B}^{\text{ext}}$ yields a force that is always perpendicular to the $\mathbf{B}^{\text{ext}}$ field and subsequently will traverse a path that is perpendicular to $\mathbf{B}^{\text{ext}}$. Initially, the particles will rotate around the $\mathbf{B}^{\text{ext}}$-axis and then become stationary if there is any drag, unless there is an electric field, which will then draw the particles (or repel them) in the E-direction. The stages of evolution of the blast envelope are as follows (Fig. 2):

- The particles initially move radially-outward from the blast.
- The particles experience a magnetically-induced rotational force in $\mathbf{n} \times \mathbf{B}^{\text{ext}}$ direction, that starts a large-scale rotation about the $\mathbf{B}^{\text{ext}}$-axis. Particles that were initially blasted in the direction of the $\mathbf{B}^{\text{ext}}$-axis travel further in that direction.
- The drag forces slowly start to decay the energy of the particles, and the orbits become progressively smaller.
- The drag forces eventually absorb all the energy, and the particles cease to move.

**Remark 1.** If the particles have mixed charges, depending on their sign (negative or positive), they will swirl in clockwise of counterclockwise directions.

**Remark 2.** If other physical forces were included, such as an electric field, the particles would then draw the particles (or repel them) in the E-direction or, for example, gravity would cause the particles to settle.

### 4. Isolating the effects of drag

#### 4.1. Terminal blast radius

The differential equation for each particle in its outward normal direction is $(m_i = m)$, assuming no gravity, buoyancy or fluid velocity ($v_f = 0$)¹:

$$m \dot{v}_{in} = -\frac{1}{2} \rho_a C_D v_{in}^2 A, \quad (4.1)$$

where $v_{in}$ is the outward normal velocity, which can be written as

$$\dot{v}_{in} = -K v_{in}^2, \quad (4.2)$$

where for a sphere

$$K = \frac{1}{2m} C_D \rho_a A = \frac{3C_D \rho_a}{8\rho R}. \quad (4.3)$$

Using the chain rule

$$\frac{d v_{in}}{dt} = \frac{d v_{in}}{dr_{in}} \frac{dr_{in}}{dt} = \frac{d v_{in}}{dr_{in}} v_{in} = -K v_{in}^2, \quad (4.4)$$

which yields

$$\frac{d v_{in}}{dr_{in}} = -K v_{in}, \quad (4.5)$$

and subsequently

$$\frac{d v_{in}}{v_{in}} = -K dr_{in} \Rightarrow \int_{v_{in}}^{v_{in}(t)} \frac{d v_{in}}{v_{in}} = -\int_{r_{in}}^{r_{in}(t)} K dr_{in}. \quad (4.6)$$

¹ The subscript $n$ indicates the outward normal direction.
where \( r_{in} \) is the outward normal position, with solution
\[
v_{in}(t) = v_{oin}e^{-K(r_{in}(t) - r_{oin})},
\]
(4.7)
with inverse solution, for the blast radius
\[
R(t) = r_{in}(t) - r_{oin} = -\frac{1}{K} \ln \left( \frac{v_{in}(t)}{v_{oin}} \right) = -\frac{8\rho R}{3C_D\rho_a} \ln \left( \frac{v_{in}(t)}{v_{oin}} \right),
\]
(4.8)
where \( \frac{1}{K} \) has units of meters. This shows the explicit inverse relationship between the size of the blast radius and \( K \), which is a measure of the drag (tending to limit the blast radius growth) and the mass (tending to increase the blast radius growth). One can relate this directly to the energy of detonation and total mass via Eq. (3.4), utilizing \( v_{oin} = \sqrt{\frac{2W}{M}} \).

\[
R(t) = r_{in}(t) - r_{oin} = -\frac{8\rho R}{3C_D\rho_a} \ln \left( \frac{v_{in}(t)}{\sqrt{\frac{2W}{M}}} \right).
\]
(4.9)

**Remark.** One could directly integrate Eq. (4.2) in time to yield
\[
v_{in}(t) = \frac{v_{oin}}{Ktv_{oin} + 1} = \frac{\sqrt{\frac{2W}{M}}}{Kt\sqrt{\frac{2W}{M}} + 1},
\]
(4.10)
and
\[
r_{in}(t) = r_{oin} + \frac{1}{K} \ln (Ktv_{oin} + 1) = r_{oin} + \frac{1}{K} \ln \left( Kt\sqrt{\frac{2W}{M}} + 1 \right). \quad (4.11)
\]
One can also invert Eq. (4.11) to yield an expression for the time it takes to achieve a certain blast radius:
\[
t = \frac{e^{K(r_{in}(t) - r_{oin})} - 1}{K\sqrt{\frac{2W}{M}}}.
\]
(4.12)

### 4.2. Hybrid drag

Generally speaking, the drag coefficient, which is an empirical parameter which attempts to represent the action of the fluid forces on an object, is not a constant, and would vary with, for example, the Reynolds number. In the zero Reynolds number limit the drag would be that of a Stokesian regime. One possible way to represent the drag coefficient is with a piecewise definition, as a function of the Reynolds number (Chow [20]):

- For \( 0 < Re \leq 1 \), \( C_D = \frac{24}{Re} \),
- For \( 1 < Re \leq 400 \), \( C_D = \frac{24}{Re^{2.5}} \),
- For \( 400 < Re \leq 3 \times 10^5 \), \( C_D = 0.5 \),
- For \( 3 \times 10^5 < Re \leq 2 \times 10^6 \), \( C_D = 0.000366Re^{0.4275} \),
- For \( 2 \times 10^6 < Re < \infty \), \( C_D = 0.18 \),

where the local Reynolds number for a particle is \( Re \overset{\text{def}}{=} \frac{2\rho_a|v_f - v_p|}{\mu_f} \) and \( \mu_f \) is the fluid viscosity. The viscosity coefficient for air is \( \mu_f = 0.000018 \text{ Pa/s} \). Using the hybrid model reduces the drag at the lower Reynolds number regimes, relative to simply picking a constant mid-range value for \( C_D \) (for example \( C_D = 0.5 \)), thus producing a larger blast radius than a constant drag coefficient.
Remarks. The piecewise drag law of Chow [20] is a mathematical description for the Reynolds number over a wide range and is a curve-fit of extensive data from Schlichtling [21]. As observed in the experimental data, the mathematical function exhibits a discontinuity at $Re = 3 \times 10^5$, although in an explosion the time a particle spends at this Reynolds number is almost negligible. In the low velocity (low Reynolds number) limit a Stokesian model is most appropriate, which is what the drag law above attempts to incorporate. The drag forces are significantly smaller with a Stokesian model.

Comparing a purely Stokesian drag law, which would be valid for small particles and laminar flow (low Reynolds number)

$$
\Psi_{\text{drag,Stokesian}}^i = c(v_f - v_i) = \mu_f 6\pi R_i(v_f - v_i),
$$

where $\mu_f$ is the fluid viscosity. We observe the following:

$$
\frac{\|\Psi_{\text{drag,Stokesian}}\|}{\|\Psi_{\text{drag}}\|} = \frac{12\mu_f}{\rho_a C_D R\|v_f - v_i\|},
$$

For typical parameters for air and spherical particles (using $C_D = 0.5$, which is a mid-range value from the piecewise drag law introduced earlier), we have

$$
\frac{\|\Psi_{\text{drag,Stokesian}}\|}{\|\Psi_{\text{drag}}\|} \approx 0.0004 R\|v_f - v_i\|,
$$

which indicates that for extremely small particles and low velocities, the Stokesian model dominates, while for larger particles and large velocities, the phenomenological model dominates. Appendix A illustrates blast results using a Stokesian model.

5. Comparative contributions of electromagnetic forces to drag

Consider a drag force is given by:

$$
\Psi_{\text{drag}} = C_D \frac{1}{2} A \rho_f \|v_f - v\|^2 \tau,
$$

where

$$
\tau \overset{\text{def}}{=} \frac{v_f - v}{\|v_f - v\|},
$$

and $A = \pi R^2$, where $R$ is the particle radius. In order to determine the relative strengths of the fluid drag force to the electromagnetic forces acting on the particle, consider the following model for an isolated particle:

$$
m \dot{v} = \Psi_{\text{drag}} + \Psi_{e+m} = C_D \frac{1}{2} A \rho_f \|v_f - v\|^2 \tau + \bar{q} \rho_p V (E^{\text{ext}} + v \times B^{\text{ext}}),
$$

where $\bar{q}$ is the charge per unit mass, $\rho_p$ is the density of the particle and $V = \frac{4}{3} \pi R^3$. The general ratio is

$$
\lambda(v) \overset{\text{def}}{=} \frac{\|\Psi_{e+m}\|}{\|\Psi_{\text{drag}}\|} = \frac{\|\bar{q} \rho_p V (E^{\text{ext}} + v \times B^{\text{ext}})\|}{C_D \frac{1}{2} A \rho_f \|v_f - v\|^2} = \frac{8|\bar{q}| \rho_p R}{3C_D \rho_f} \left( \frac{\|E^{\text{ext}} + v \times B^{\text{ext}}\|}{\|v_f - v\|^2} \right).
$$

Using the Triangle and Cauchy–Schwarz inequalities:

$$
\lambda(v) \leq \frac{8|\bar{q}| \rho_p R}{3C_D \rho_f} \left( \frac{\|E^{\text{ext}}\| + \|v\|\|B^{\text{ext}}\|}{\|v_f - v\|^2} \right),
$$

which leads to

$$
\|E^{\text{ext}}\| + \|v\|\|B^{\text{ext}}\| \geq \lambda(v) \frac{3C_D \rho_f \|v_f - v\|^2}{8|\bar{q}| \rho_p R}.
$$
If we set $\lambda = 1$, we obtain an expression for the electromagnetic forces to have parity with the drag force. In the case when the magnetic field is negligible, we have:

$$\|E^\text{ext}\| = \frac{3C_D \rho f \|v_f - v\|^2}{8|\bar{q}|\rho_p R}.$$  \hspace{1cm} (5.7)

In the case when the electric field is negligible, we have

$$\|B^\text{ext}\| \geq \frac{3C_D \rho f \|v_f - v\|^2}{8|\bar{q}|\rho_p R}.$$  \hspace{1cm} (5.8)

6. A numerical example for non-interacting particles

The previous expressions provide a qualitative guide measure of the relative force contributions that particles encounter in such regimes. However, to solve the governing equation, when electromagnetic effects are included

$$m \dot{v}_i = \Psi_{\text{drag}}^i + \Psi_{\text{em}}^i = \frac{1}{2} \rho_a C_D \|v_f - v_i\|(v_f - v_i)A + q(E^\text{ext} + v \times B^\text{ext})$$ \hspace{1cm} (6.1)

we integrate the governing equations numerically

$$v_i(t + \Delta t) = v_i(t) + \frac{1}{m} \int_t^{t + \Delta t} (\Psi_{\text{drag}}^i + \Psi_{\text{em}}^i) \, dt$$

$$\approx v_i(t) + \frac{\Delta t}{m_i} \left( \Psi_{\text{drag}}^i(t) + \Psi_{\text{em}}^i(t) \right).$$ \hspace{1cm} (6.2)

6.1. Simulation

In order to illustrate the model, the following simulation parameters were chosen (they are not intended to simulate a specific blast event):

- Magnetic field, $B^\text{ext} = (10, 0, 0)$ T,
- Electric field, $E^\text{ext} = (0, 0, 0)$ N/C,
- Charge per unit mass, $q = 10$ C/kg,
- Total simulation duration, 1 s,
- The time step size, $\Delta t = 10^{-4}$ s,
- Detonation energy, $W = 10,000$ J,
- Density of air, $\rho_a = 1.225$, kg/m$^3$,
- Particles were distributed randomly in a spherical starting radius, $R(t = 0) = 1$ m,
- Number of particles, $N = 2000$,
- Radius of particles, $R_i = 0.05$ m and
- Density of blast material, $\rho = 7000$ kg/m$^3$.

An extremely small (relative to the total simulation time) time-step size of $\Delta t = 10^{-4}$ s was used. Further reductions of the time-step size produced no noticeable changes in the results, thus the solutions generated can be considered to have negligible numerical error. The simulations took under one minute on a standard laptop. Fig. 5 illustrates the results for the parameters above. For comparison Fig. 7 illustrates the results with no magnetic field. As the figures indicate, an ellipsoidal blast evolves due to the induced cyclotron radii that evolve for each particle, with orbits around the $B^\text{ext}$-field axis. For more general blast conditions, there can be cases where the interaction between the particles, for example particle $i$ and particle $j$, $\Psi_{ij}(t)$, may be important, for example due to near-field interaction and/or contact. Fig. 6 illustrates the evolving configuration with velocity vectors shown and corresponding plots of the $x_2$ and $x_3$ velocities as a function of time. The ratio of the electromagnetic (in this case purely magnetic) forces at $v(t = 0)$ (using $C_D = 1$ for illustration purposes here only) is (from Eq. (5.8))
\[ \frac{\| \Psi^{e+m} \|}{\| \Psi^{drag} \|} = \lambda(v(t = 0)) \approx 56504.7, \]  
indicating that drag plays a very small role in for this set of parameters in the magnetic rotation phase of the dynamics. This is also reflected in the virtually zero outward expansion of the particle in the \( x_2 - x_3 (y - z) \) equatorial plane dynamics (Fig. 5).

6.2. Particle interactions

Had the particle noninteraction approximation not been invoked, a coupled system of equations would arise due to the interaction between the particles. For example, this entails numerically integrating the governing equations, which leads to (for example using a trapezoidal rule with variable integration metric, \( 0 \leq \phi \leq 1 \))

\[ v_i(t + \Delta t) = v_i(t) + \frac{1}{m_i} \int_t^{t+\Delta t} (\Psi_i^{drag} + \sum_{j=1,j\neq i}^K \Psi_{ij} + \Psi_i^{e+m}) \, dt \]

\[ \approx v_i(t) + \Delta t \phi \left( \Psi_i^{drag}(t + \Delta t) + \sum_{j=1,j\neq i}^K \Psi_{ij}(t + \Delta t) + \Psi_i^{e+m}(t + \Delta t) \right) \]

\[ + \frac{\Delta t (1 - \phi)}{m_i} \left( \Psi_i^{drag}(t) + \sum_{j=1,j\neq i}^K \Psi_{ij}(t) + \Psi_i^{e+m}(t) \right), \]  
(6.4)

where \( \Psi_{ij}(t) \) represents particle \( i \)'s interaction with the neighboring \( j = 1, 2, \ldots, N \) particles. The position can be computed via application of the trapezoidal rule again:

\[ r_i(t + \Delta t) \approx r_i(t) + \Delta t (\phi v_i(t + \Delta t) + (1 - \phi)v_i(t)), \]  
(6.5)

which can be consolidated into

\[ r_i(t + \Delta t) = r_i(t) + v_i(t) \Delta t \]

\[ + \frac{\phi^2 (\Delta t)^2}{m_i} \left( \Psi_i^{drag}(t + \Delta t) + \sum_{j=1,j\neq i}^K \Psi_{ij}(t + \Delta t) + \Psi_i^{e+m}(t + \Delta t) \right) \]

\[ + \frac{(1 - \phi)(\Delta t)^2}{m_i} \left( \Psi_i^{drag}(t) + \sum_{j=1,j\neq i}^K \Psi_{ij}(t) + \Psi_i^{e+m}(t) \right). \]  
(6.6)

This leads to a coupled set of equations. We now discuss the details of this formulation further.

7. Particle-interaction models

In order to represent the group of interacting particles, we follow a relatively flexible formulation found in Zohdi [12–17]. We consider a group of non-intersecting particles \( (i = 1, 2, \ldots, N_p) \). The objects in the system are assumed to be small enough to be considered (idealized) as particles, spherical in shape, and that the effects of their rotation with respect to their mass center is unimportant to their overall motion, although, we will make further remarks on these effects shortly. The equation of motion for the \( i \)th particle in system is

\[ m_i \ddot{r}_i = \Psi_i^{tot}(r_1, r_2, \ldots, r_{N_p}) = \Psi_i^{con} + \Psi_i^{bond} + \Psi_i^{drag} + \Psi_i^{e+m}, \]  
(7.1)

where \( r_i \) is the position vector of the \( i \)th particle and where \( \Psi_i^{tot} \) represents all forces acting on particle \( i \), which is decomposed into the sum of forces due to:

- Inter-particle forces \( (\Psi_i^{con}) \) generated by contact with other particles,
- Possible adhesive bonding forces \( (\Psi_i^{bond}) \) with other particles,
These forces include:

- Drag forces arising from the surrounding environment ($\Psi_{\text{drag}}$),
- Near-field interaction and external electromagnetic forces ($\Psi_{\text{e}+m}$).

In the next sections, we examine each of the types of forces in the system in detail.

### 7.1. Particle-to-particle contact forces

Following Zohdi [12–17], we employ a simple particle overlap model to determine the normal contact force contributions from the surrounding particles ($N_{\text{ci}}$) in contact, $\Psi_{\text{con},n} = \sum_{j=1}^{N_{\text{ci}}} \Psi_{\text{con},n,ij}$, based on separation distance between particles in contact (Fig. 3). Generally,

$$\Psi_{\text{con},n,ij} = \mathcal{F}(\|r_i - r_j\|, R_i, R_j, \text{material parameters}).$$

(7.2)

There is no shortage of contact models, of varying complexity, to generate a contact interaction force. Throughout this work, we will utilize a particularly simple relation whereby contact force is proportional to the relative normalized proximity of particles $i$ and $j$ in contact, detected by the distance between centers being less that the sum of the radii

If $\|r_i - r_j\| \leq R_i + R_j \Rightarrow$ activate contact,

(7.3)

where we define the overlap as

$$\delta_{ij} \overset{\text{def}}{=} \|r_i - r_j\| - (R_i + R_j).$$

(7.4)

Accordingly, we consider the following

$$\Psi_{\text{con},c} \propto -K_{pj}|\mathcal{E}_{ij}|^{p_p}n_{ij}A_{ij}^c,$$

(7.5)

where $0 < K_{pj} < \infty$ is a particle-to-particle contact compliance constant, $p_p$ is a material parameter, $\mathcal{E}_{ij}$ is normalized/nondimensional (strain-like) deformation metric

$$\mathcal{E}_{ij} = \left| \frac{\|r_i - r_j\| - (R_i + R_j)}{(R_i + R_j)} \right| = \frac{\delta_{ij}}{(R_i + R_j)}$$

(7.6)

and

$$n_{ij} = \frac{r_i - r_j}{\|r_i - r_j\|} = \frac{r_j - r_i}{\|r_i - r_j\|},$$

(7.7)

where the $R_i$ and $R_j$ are the radii of particles $i$ and $j$ respectively. The term $A_{ij}^c$ is a contact area parameter, which is discussed in Appendix B. Appendix B also provides a brief review of alternative models, such as the classical Hertzian contact model.
7.2. Comments on rolling/spinning

The introduction of rolling and spin is questionable for a small object, idealized by a particle, in particular because of rolling resistance. In addition to the balance of linear momentum, \( m_i \dot{v}_i = \Psi_i^\text{tot} \), where the \( v_i \) is the velocity of the center of mass, the equations of angular momentum read

\[
\dot{H}_{i,cm} = \frac{d(I_i \omega_i)}{dt} = M_i^\text{tot}_{i,cm}.
\]

For spheres, we have

\[
H_{i,cm} = \Gamma_{i,s} \omega_i = \frac{2}{5} m_i R_i^2 \omega_i
\]

and for the time discretization

\[
\omega_i(t + \Delta t) = \omega_i(t) + \frac{\Delta t}{\Gamma_{i,s}} \left( \phi M_i^\text{tot}_{i,cm}(t + \Delta t) + (1 - \phi)M_i^\text{tot}_{i,cm}(t) \right),
\]

where \( M_i^\text{tot}_{i,cm} \) are the total moments generated by interaction forces, such as contact forces and rolling resistance. For the applications at hand, the effects of rolling is generally negligible, in particular because the particles are small. However, nonetheless, we formulate the system with rotations where \( r_i \) is the position of the center of mass, \( v_i \) is the velocity of the center of mass and \( \omega_i \) is the angular velocity. An important quantity of interest is the velocity on the surface of the “particles”, which is a potential contact point with other particles, denoted \( v_i^c \)

\[
v_i^c = v_i + \omega_i \times r_{i \rightarrow c},
\]

where \( r_{i \rightarrow c} \) is the relative position vector from the center to the possible point of contact. This is utilized further later.

7.3. Contact dissipation

Phenomenological particle contact dissipation can be incorporated by tracking the relative velocity of the particles in contact. A simple model to account for this is

\[
\Psi_{ij}^\text{con,d} = c^{cd} (v_{j,n} - v_{i,n}) A^c_{ij},
\]

where \( c^{cd} \) is a contact dissipation parameter.

7.4. Regularized contact friction models

Frictional stick is modeled via the following regularized friction algorithm: (at the point of contact)

- Check static friction threshold \( (K_f^s \) is a tangential contact friction compliance constant):

\[
K_f^s \|v_{j,t}^c - v_{i,t}^c\| A^c_{ij} \Delta t \quad \text{against} \quad \mu_s \|\Psi_{ij}^\text{con,n}\|,
\]

where \( \|v_{j,t}^c - v_{i,t}^c\| \Delta t \) is the relative tangential velocity at a point of contact, \( \Delta t \) is the time-step used later in the numerical discretization.\(^2\) \( \mu_s \) is the static friction coefficient. This step replaces (“regularizes”) a more rigorous, and difficult, step of first assuming no slip, generating the no-slip contact forces, by solving an entire multibody/multisurface contact problem, \( \Psi_{ij}^\text{ns} \), and checking \( \Psi_{ij}^\text{ns} \) against the threshold \( \mu_s \|\Psi_{ij}^\text{con,n}\| \) on each surface.

- If the threshold is not met \( (K_f^s \|v_{j,t}^c - v_{i,t}^c\| A^c_{ij} \Delta t < \mu_s \|\Psi_{ij}^\text{con,n}\|) \), then

\[
\Psi_{ij}^\text{con,f} = K_f^s \|v_{j,t}^c - v_{i,t}^c\| A^c_{ij} \Delta t \tau_{ij}^c
\]

where

\[
\tau_{ij}^c = -\frac{v_{j,t}^c - v_{i,t}^c}{\|v_{j,t}^c - v_{i,t}^c\|} = \frac{v_{j,t}^c - v_{i,t}^c}{\|v_{j,t}^c - v_{i,t}^c\|},
\]

where the subscripts indicate the tangential components of velocity. The tangential velocity at the contact point is obtained by subtracting away the normal component of the velocity

\[
v_i^c = v^c - (v^c \cdot n)n.
\]

\(^2\) The product, \( \|v_{j,t}^c - v_{i,t}^c\| \Delta t \) has dimensions of length.
• If the threshold is met or exceeded ($K_f \|v_j^e - v_i^e\|A_{ij}^c \Delta t \geq \mu_s \|\Psi^{con,n}\|$), then one adopts a slip model of the form
$$\Psi^{con,f}_{ij} = \mu_d \|\Psi^{con,n}_{ij}\| \tau_{ij}^c,$$
where $\mu_d$ is the dynamic friction coefficient.

7.5. Particle-to-particle bonding relation

For the particles to bond, we adopt a criterion based on exceeding a critical interpenetration distance. Explicitly:
• Recall, if $\|r_i - r_j\| \leq (R_i + R_j)$, then the particles are in contact and $E_{ij} = \frac{\delta_{ij}}{(R_i + R_j)}$.
• If the particles are in contact and $|E_{ij}| \geq E^*$, then an (adhesive/attractive) normal bond is activated between the particles of the form
$$\Psi^{bond,n}_{ij} = K_{nb}^i |\Psi^{con,n}_{ij}|^p_b n_{ij} A_{ij}^c,$$
where $0 \leq K_{nb}^i$ is a bonding constant and $p_b$ is a material parameter.
• If the particles have an activated normal bond, then the particles automatically have a rotational/tangential bond equivalent in form to stick friction
$$\Psi^{bond,r}_{ij} = K_f^j \|v_j^e - v_i^e\|A_{ij}^c \Delta t \tau_{ij}^r.$$ (7.17)

We note the choices of the values of the coefficients and exponents are given later in the paper when a numerical example is given.

Remark. Although thermal effects were not considered, the algorithm can be modified to account for coupled thermal effects. In those cases, the parameters, such as $K_{p_{ij}}$ can be thermally dependent since the particles can thermally soften. For example, the compliance constant for the particles in the contact law can be written as (here $\Theta$ is the temperature, which is fixed in the present analysis):
$$K_{pi} = \text{MAX} \left( K_{pio} \left( e^{-a_i \left( \frac{\Theta}{\Theta_i} - 1 \right)} \right), K_{lim_{pi}} \right),$$ (7.18)
and for particle $j$
$$K_{pj} = \text{MAX} \left( K_{pjo} \left( e^{-a_j \left( \frac{\Theta}{\Theta_j} - 1 \right)} \right), K_{lim_{pj}} \right).$$ (7.19)
and take the average at the interface and the value in the contact law:
$$K_{p_{ij}} = \frac{1}{2} \left( K_{pi} + K_{pj} \right).$$ (7.20)

There is a multitude of possible representations, and it is relatively easy to select one or the other, and to embed in the staggering framework developed. A fully coupled thermal model is not considered here, and we refer the reader to Zohdi [12–17] for more details in that direction.

7.6. Surrounding and interstitial drag

Finally, we note that drag from the interstitial and surrounding fluid (or even smaller-scale particles, solvents) will be accounted for by the previously discussed drag model
$$\Psi_i^{drag} = \frac{1}{2} \rho_a C_D \|v^f - v_i\| (v^f - v_i) A_i,$$ (7.21)
where $C_D$ is the drag coefficient, $A_i$ is the reference area, which for a sphere is $A_i = \pi R_i^2$, $\rho_a$ is the density of the ambient fluid environment and $v^f$ is the velocity of the surrounding medium. We will assume that the local average surrounding velocity be $v^e \approx 0$, for most applications of interest presently.
7.7. Near-field/electromagnetic forces

Following Zohdi [12–17], the electromagnetic forces are decomposed into three contributions, (1) Lorentz forces (for charged particles), (2) inter-particle near-field forces, (3) magnetic forces (for magnetic particles) and

\[
\Psi_i^{e+m} = \Psi_i^{lor,e+m} + \Psi_i^{mag} + \sum_{j \neq i}^{N} \Psi_{ij}^{nf} = q_i (E_{ext}^{ext} + v_i \times B_{ext}^{ext}) + \Psi_i^{nf} + \Psi_i^{mag},
\]

(7.22)

where \(\sum_{j \neq i}^{N} \Psi_{ij}^{nf}\) represents the interaction between particle \(i\) and all other particles \(j = 1, 2...N (j \neq i)\). \(\Psi_i^{lor,e+m}\) represents external Lorentz-induced forces from the surrounding environment, for example comprised of \(E_{ext}\) and \(B_{ext}\), which are externally-controlled fields that are independent of the response of the system. The terms \(E_{ext}\) and \(B_{ext}\) can be considered as static (or extremely slowly-varying), and thus mutually uncoupled and independently controllable. The self-induced magnetic fields developed between particles is insignificant (Jackson [11]) for the velocity ranges of interest here (well below the speed of light). Following Zohdi [12–17], a simple form that captures the essential near-field effects is

\[
\Psi_i^{nf} = \sum_{i \neq j}^{N_p} \left( \frac{\alpha_{1ij} \|r_i - r_j\|^{-\beta_1} - \alpha_{2ij} \|r_i - r_j\|^{-\beta_2}}{\text{attraction}} \right) n_{ij},
\]

(7.23)

where the \(\alpha\)'s and \(\beta\)'s are empirical material parameters. The various representations (decompositions) of the coefficients that appear in Eq. (7.23) are with \(c_i = \pm 1\) (a positive/negative identifier): (a) mass-based \((m = mass)\): \(\alpha_{ij} = \tilde{\alpha}_{ij} m_i c_i c_j\), (b) surface area-based \((a = surface\) area): \(\alpha_{ij} = \tilde{\alpha}_{ij} a_i a_j c_i c_j\), (c) volume-based \((V = volume)\): \(\alpha_{ij} = \tilde{\alpha}_{ij} V_i V_j c_i c_j\) and (d) charge-based: \(\alpha_{ij} = \tilde{\alpha}_{ij} q_i q_j c_i c_j\), where the \(\tilde{\alpha}_{ij}\) are empirical material parameters. There are vast numbers of empirical representations, for example, found in the field of “Molecular Dynamics” (MD), which typically refers to mathematical models of systems of atoms or molecules where each atom (or molecule) is represented by a material point and is treated as a point mass. The overall motion of such mass-point systems is dictated by Newtonian mechanics. For an extensive survey of MD-type interaction forces, which includes comparisons of the theoretical and computational properties of a variety of interaction laws, we refer the reader to Frenklach and Carmer [22]. In the usual MD approach (see Haile [23], for example), the motion of individual atoms is described by Newton’s second law with the forces computed from differentiating a prescribed potential energy function, with applications to solids, liquids, and gases, as well as biological systems (Hase [24], Schlick [21] and Rapaport [25]). The interaction functions usually take the form of the familiar Mie, Lennard-Jones, and Morse potentials (Moelwyn-Hughes [26]), however three-body terms can be introduced directly into the interaction functions (Stillinger [27]) or, alternatively, “local” modifications can be made to two-body representations (Tersoff [28]).

Remark. Although we will ignore magnetic particle effects in the upcoming analysis, we mention that an additional force can be exerted on magnetic particles, independent of the electrodynamically-induced Lorentz forces. A relatively simple model for the characterization of this force is given by

\[
\Psi^{mag} = \nabla (\gamma B_{ext}^{ext} \cdot B_{ext}^{ext}),
\]

(7.24)

where \(\gamma\) is a material parameter that is related to the magnetization of the particle, and which is dependent on the magnetic dipole properties, the magnetic susceptibility, the magnetic permeability and the internal magnetic moment density of the material (see Feynman et al. [29], Cullity and Graham [30], Boyer [31] or Jackson [11]).

8. System time-stepping for systems of interacting particles

Integrating Eq. (7.1) leads to (using a trapezoidal rule with variable integration metric, \(0 \leq \phi \leq 1\))

\[
v_i(t + \Delta t) = v_i(t) + \frac{1}{m_i} \int_t^{t+\Delta t} \Psi_i^{tot} \, dt
\]
\[
\approx v_i(t) + \frac{\Delta t}{m_i} \left( \phi \Psi_i^{tot}(t + \Delta t) + (1 - \phi) \Psi_i^{tot}(t) \right),
\]
(8.1)

where \( \Psi_i^{tot} = \Psi_i^{con} + \Psi_i^{bond} + \Psi_i^{drag} + \Psi_i^{e+m} \). The position can be computed via application of the trapezoidal rule again:

\[
r_i(t + \Delta t) \approx r_i(t) + \Delta t \left( \phi v_i(t + \Delta t) + (1 - \phi) v_i(t) \right),
\]
(8.2)

which can be consolidated into

\[
r_i(t + \Delta t) = r_i(t) + \Delta t \left( \phi \Psi_i^{tot}(t + \Delta t) + (1 - \phi) \Psi_i^{tot}(t) \right).
\]
(8.3)

This leads to a coupled system of equations, which are solved using an adaptive iterative scheme, building on approaches found in various forms in Zohdi [12–17].

### 8.1. Iterative (implicit) solution method-algorithm

Following the basic framework in Zohdi [12–17], we write Eq. (8.3) in a slightly more streamlined form for particle \( i \)

\[
r_i^{L+1} = r_i^L + v_i^L \Delta t + \frac{\phi (\Delta t)^2}{m_i} \left( \phi (\Psi_i^{tot,L+1}) + (1 - \phi) (\Psi_i^{tot,L}) \right),
\]
(8.4)

which leads to a coupled set equations for \( i = 1, 2, \ldots, N_p \) particles, where the superscript \( L \) is a time interval counter. Appendix C provides details on this solution process. The solution steps are, within a time-step:

- (1): Start a global fixed iteration (set \( i = 1 \) (particle counter) and \( K = 0 \) (iteration counter))
- (2): If \( i > N_p \) then go to (4)
- (3): If \( i \leq N_p \) then:
  - (a) Compute the position \( r_i^{L+1,K} \)
  - (b) Go to (2) for the next particle \( (i = i + 1) \)
- (4): Measure error (normalized) quantities
  - (a) \( \sigma_K \) def \( = \frac{\sum_{i=1}^{N_p} ||r_i^{L+1,K} - r_i^{L+1,K-1}||}{\sum_{i=1}^{N_p} ||r_i^{L+1,K} - r_i^L||} \)
  - (b) \( Z_K \) def \( = \frac{\sigma_K}{TOL} \)
  - (c) \( A_K \) def \( = \frac{\left( \frac{r_i^{tot}}{\sigma_K} \right)^{1/2}}{\left( \frac{r_i^{old}}{\sigma_K} \right)^{1/2}} \) (see Appendix C)
- (5): If the tolerance is met: \( Z_K \leq 1 \) and \( K < K_d \) then
  - (a) Increment time: \( t = t + \Delta t \)
  - (b) Construct the next time step: \( (\Delta t)^{new} = A_K (\Delta t)^{old} \)
  - (c) Select the minimum size: \( \Delta t = \text{MIN}((\Delta t)^{lim}, (\Delta t)^{new}) \)
  - (d) Update the ray positions and go to (0)
- (6): If the tolerance is not met: \( Z_K > 1 \) and \( K < K_d \) then
  - (a) Update the iteration counter: \( K = K + 1 \)
  - (b) Reset the particle counter: \( i = 1 \)
  - (c) Go to (2)
- (7): If the tolerance is not met \( (Z_K > 1) \) and \( K = K_d \) then
  - (a) Construct a new time step: \( (\Delta t)^{new} = A_K (\Delta t)^{old} \)
  - (b) Restart at time \( t \) and go to (1).

Time-step size adaptivity is critical, since the system’s dynamics and configuration can dramatically change over the course of time, possibly requiring quite different time step sizes to control the iterative error. However, to maintain the accuracy of the time-stepping scheme, one must respect an upper bound dictated by the discretization error, i.e., \( \Delta t \leq \Delta t^{lim} \). Note that in step (5), \( A_K \) may enlarge the time-step if the error is lower than the preset tolerance.
9. Numerical examples for systems of interacting particles

As an example, we consider a group of \( N_p \) randomly dispersed spherical particles, of equal size, generated within a spherical (aggregate) domain of diameter \( D \). The ratio of particle diameter, \( d \), to total domain diameter, \( D \), was \( d/D = 0.05 \). In order to generate the random particle positions, the classical random sequential addition (RSA) algorithm was used to place nonoverlapping particles into the domain of interest (Widom [32]), initially a sphere, which was then allowed to dynamically converge to an equilibrium state.\(^3\) The following relevant other simulation parameters chosen were (in SI-units if not explicitly stated), in addition to the parameters provided earlier:

- The normal contact parameter was \( K_{p_0} = 10^7 \text{ N/m}^2 \), at a fixed temperature, \( K_p = \text{MAX}(K_{p_0} \left( e^{-\frac{\Theta}{\Theta^*} - 1} \right) , K_{p_{\text{lim}}}) \), where \( \Theta^* = 500 ^\circ \text{K}, K_{p_{\text{lim}}} = 10^8 \text{ N/m}^2 \), the exponent in the contact law was set to \( p_p = 2 \), the temperature was fixed to be \( \Theta = 300 ^\circ \text{K} \) and the thermal sensitivity parameter was set to \( a = 1 \),
- The contact damping parameter, \( c^c_d = 10^5 \),
- The friction contact parameter \( K_f = 10^7 \),
- The coefficient of static friction, \( \mu_s = 0.4 \),
- The coefficient of dynamic friction, \( \mu_d = 0.3 \),
- The normal bond parameter, \( K^{\text{nb}} = 10^6 \text{ N/m}^2 \) and the exponent in the binding law was set to \( p_b = 2 \),
- The rotational/tangential bond parameter, \( K^{\text{tb}} = 10^3 \),
- The nearfield parameters, \( \tilde{\alpha}_1 = 0.5, \beta_1 = 1, \tilde{\alpha}_2 = 0.01, \beta_2 = 2 \), where the \( \tilde{\alpha} \) is per unit mass,
- The target number of fixed point iterations, \( K_d = 10 \),
- The trapezoidal time-stepping parameter, \( \phi = 0.5 \),
- The initial time step size, \( 0.00001 \text{ s} \),
- The time step upper bound, \( 0.00025 \text{ s} \) and
- The tolerance for the fixed-point iteration, \( 5 \times 10^{-4} \).

The sequence in Fig. 8 illustrates the effects when the particles interact through contact only, while the sequence in Fig. 9 illustrates the effects with contact and near-field effects. The results in Fig. 8 indicate that contact alone is of minimal importance, primarily because of the predominately radially-outward motion of the initial blast, where the particles essentially follow one another. However, Fig. 9 illustrates that nearfield effects allow “agglomeration” forming a “clumpy helix”.

10. Summary, conclusions and extensions

For general blast conditions, there can be cases where the change in the surrounding fluid’s behavior due to the motion of the particles, may be important. This yields a coupled system of equations for the interaction between the particles and the fluid, which would necessitate spatio-temporal discretization for example using Finite Element, Finite Difference, Finite Volume or Discrete Element Methods, such as those found in Onate et al. [40,41], Avci and Wriggers [19], Leonardi et al. [42], Onate et al. [43], Bolintineanu et al. [44] and Zohdi [12–17]. Furthermore, in order to obtain more accurate initial conditions for the system, advanced models would also involve detailed modeling of the initial packing of the material (Zohdi [45,46]), and the evolution of heat and the mechanics of the surrounding fluid environment. Such systems are quite complex. Thus, in order to qualitatively understand such systems a priori, the results presented in this paper are useful. In this vein, a closely related class of electromagnetically sensitive fluids are Ferrofluids, which are colloidal liquids of ferromagnetic nanoscale (10 nm or less) particles, often from an iron-based compound, such as magnetite or hematite, usually in an organic solvent. The volume fraction of the particles is typically under 5 percent by volume. The particles are usually coated with a surfactant (typically Oleic acid, citric acid, soy lecitin, tetramethylammonium hydroxide) to avoid agglomeration. The surfactant is strong enough to counteract near-field interaction effects between particles. The particles usually do not retain magnetization and can be considered as paramagnetic. Furthermore, they lose their magnetic properties at sufficiently high (Curie) temperatures.\(^4\) We refer the reader to Albrecht et al. [47], Andelman and Rosensweig [48] and Berger et al. [49] for reviews. Such systems are currently under investigation by the author.

\(^3\) See Torquato [33] and Torquato and coworkers (see, for example, Kansaal et al. [34] and Donev et al. [35–39]) for a detailed review of particle packing algorithms.

\(^4\) Another class of electromagnetically sensitive particle laden fluid are magnetorheological fluids which are seeded with micron-sized particles, and consequently the particles can sediment over time.
Appendix A. Stokesian model

Using a Stokesian model yields, the differential equation for each particle is \( m_i \frac{dv_i}{dt} = c(v_f - v_i) \), \( \text{m.1} \)

and can be solved analytically in the normal direction \( (n_{ri}) \) to yield

\[
v_{in}(t) = (v_{in}(0) - v_{in}^-) e^{-\frac{c}{m} t} + v_{in}^+.
\] \( \text{A.2} \)

The position in the normal direction is

\[
r_{in}(t) = r_{in}(0) + A_{in} \frac{m}{c} (1 - e^{-\frac{c}{m} t}) + D_{in} t
\] \( \text{A.3} \)

where \( A_{in} = v_{in}(0) - v_{in}^- \) and \( D_{in} = v_{in}^+ \). We note that

\[
\frac{m}{c} = \frac{2R^2 \rho}{9\mu_f}.
\] \( \text{A.4} \)

In the normal direction, with \( v_f = 0 \) this collapses to a particularly simple expression for the velocity of each particle

\[
v_{in}(t) = v_{in}(0) e^{-\frac{c}{m} t}
\] \( \text{A.5} \)

and for the position, we have

\[
r_{in}(t) = r_{in}(0) + v_{in}(0) \frac{m}{c} (1 - e^{-\frac{c}{m} t})
\] \( \text{A.6} \)

To extract the blast radius

\[
v_{in}(t) = v_{in}(0) e^{-\frac{c}{m} t} = \| \delta v_{in}(0) \| e^{-\frac{c}{m} t}
\] \( \text{A.7} \)

and for the position, we have

\[
r_{in}(t) = r_{in}(0) + v_{in}(0) \frac{m}{c} (1 - e^{-\frac{c}{m} t}) = r_{in}(0) + \| \delta v_{in}(0) \| \frac{m}{c} (1 - e^{-\frac{c}{m} t})
\] \( \text{A.8} \)

Utilizing Eq. (3.4) yields

\[
v_{in}(t) = \left( \frac{2W}{M} \right) e^{-\left( \frac{9\mu_f}{2R^2 \rho} \right) t}
\] \( \text{A.9} \)
Fig. 5. Particle-to-particle noninteraction model with magnetic field: From left to right and top to bottom: progressive evolution of a blast of charged particles in the presence of a magnetic field.
and

\[ r_{in}(t) = r_{in}(0) + \left( \sqrt{\frac{2W}{M} \frac{2\rho R^2}{9\mu f}} \right) (1 - e^{-\left( \frac{9\mu_f}{2\rho^2\mu_f} \right)t}). \]  
(A.10)

We define the blast radius

\[ R(t) \overset{\text{def}}{=} r_{in}(t) - r_{in}(0) = \left( \sqrt{\frac{2W}{M} \frac{2\rho R^2}{9\mu f}} \right) (1 - e^{-\left( \frac{9\mu_f}{2\rho^2\mu_f} \right)t}). \]  
(A.11)

The maximum radius \((t = \infty)\) is

\[ R(t = \infty) = \left( \sqrt{\frac{2W}{M} \frac{2\rho R^2}{9\mu f}} \right). \]  
(A.12)

The ratio of the radius at any given time to the maximum is

\[ \frac{R(t)}{R_{\infty}} = 1 - e^{-\left( \frac{9\mu_f}{2\rho^2\mu_f} \right)t}. \]  
(A.13)

To determine the time for the blast radius to achieve a certain size, \(R(t^*) = R^*\), we may solve for the time from the above

\[ t^* = -\frac{2\rho R^2}{9\mu_f} Ln\left( \frac{R(\infty) - R^*}{R(\infty)} \right). \]  
(A.14)

The key observations are the exponential (decay-type) growth of the cloud, controlled by the amount of energy in the detonation and the ratio of the surrounding damping and the particle masses. The growth of the blast sphere is exponential, and is controlled by the ratio of the inertial and drag forces, \(\frac{2R^2\rho}{9\mu_f}\). The size of the blast sphere is proportional to the square of the size of the particles, the square-root of the stored detonation energy, inversely proportional to the square-root of the mass and inversely proportional to the viscosity of the atmosphere.
Fig. 7. Particle-to-particle noninteraction model without magnetic field: From left to right and top to bottom: progressive evolution of particles without a magnetic field.
Fig. 8. Particle-to-particle contact interaction model with magnetic field: From left to right and top to bottom: progressive evolution of charged particles in a magnetic field with only mutual contact interaction.
Fig. 9. Particle-to-particle all interaction model with magnetic field: From left to right and top to bottom: progressive evolution of charged particles in a magnetic field with both mutual contact and near-field interaction.
Appendix B. Contact area parameter and alternative models

B.1. Contact area parameter

Following Zohdi [12–17], and referring to Fig. 4, one can solve for an approximation of the common contact radius \(a_{ij}\) (and the contact area, \(A_{ij}^c = \pi a_{ij}^2\)) by solving the following three equations,

\[
a_{ij}^2 + L_i^2 = R_i^2,
\]

and

\[
a_{ij}^2 + L_j^2 = R_j^2,
\]

and

\[
L_i + L_j = \|r_i - r_j\|,
\]

where \(R_i\) is the radius of particle \(i\), \(R_j\) is the radius of particle \(j\), \(L_i\) is the distance from the center of particle \(i\) and the common contact interpenetration line and \(L_j\) is the distance from the center of particle \(j\) and the common contact interpenetration line, where the extent of interpenetration is

\[
\delta_{ij} = R_i + R_j - \|r_i - r_j\|.
\]

The above equations yield an expression \(a_{ij}\), which yields an expression for the contact area parameter

\[
A_{ij}^c = \pi a_{ij}^2 = \pi (R_i^2 - L_i^2),
\]

where

\[
L_i = \frac{1}{2} \left( \|r_i - r_j\| - \frac{R_i^2 - R_j^2}{\|r_i - r_j\|} \right).
\]

B.2. Alternative models

One could easily construct more elaborate relations connecting the relative proximity of the particles and other metrics to the contact force, \(\Psi_{ij}^{\text{con,n}} \propto F(r_i, r_j, n_{ij}, R_i, R_j, \ldots)\), building on, for example, Hertzian contact models.

This poses no difficulty in the direct numerical method developed. For the remainder of the analysis, we shall use the deformation metric in Eq. (7.6). For detailed treatments, see Wellman et al. [50–54] and Avci and Wriggers [19]. We note that with the appropriate definition of parameters, one can recover Hertz, Bradley, Johnson–Kendel–Roberts, Derjaguin–Muller–Toporov contact models. For example, Hertzian contact is widely used, with the assumptions being

- frictionless, continuous, surfaces,
- each of contacting bodies are elastic half-spaces, whereby the contact area dimensions are smaller radii of the bodies and,
- the bodies remain elastic (infinitesimal strains),

results in the following contact force:

\[
\Psi_{ij}^{\text{con,n}} = \frac{4}{3} (R^*)^{1/2} E^* \delta_{ij}^{3/2} n_{ij},
\]

which has the general form of \(\Psi^{\text{con,n}} = K_{ij}^s \delta_{ij}^p\), where

- \(R^* = \left( \frac{1}{E_i} + \frac{1}{E_j} \right)^{-1}\)
- \(E^* = \left( \frac{1-v_i^2}{E_i} + \frac{1-v_j^2}{E_j} \right)^{-1}\)
where $E$ is the Young’s modulus and $v$ is the Poisson ratio. The contact area with such a model has already been incorporated in the relation above, and is equal to $A^c_{ij} = \pi a^2$ where $a = \sqrt{R^2 \delta_{ij}}$. For more details, we refer the reader to Johnson [55]. It is obvious that for a deeper understanding of the deformation within a particle, it must be treated as a deformable continuum, which would require a highly-resolved spatial discretization, for example using the Finite Element Method for the contacting bodies. This requires a large computational effort. For the state of the art in Finite Element Methods and Contact Mechanics, see the books of Wriggers [56,57]. For work specifically focusing on the continuum mechanics of particles, see Zohdi and Wriggers [58].

Appendix C. Iterative methods

The set of equations represented by Eq. (8.4) can be solved recursively. Eq. (8.4) can be solved recursively by recasting the relation as

$$r^{L+1}_i = r^L_i + v^L_i \Delta t + \left( \frac{\phi \Delta t}{m_i} \right)^2 \psi^{\text{tot},L+1,K-1}_i + \frac{\phi (\Delta t)^2}{m_i} (1 - \phi) \psi^{\text{tot},L}_i,$$

which is of the form

$$r^{L+1}_i = \mathcal{G}(r^{L+1,K-1}_i) + L_i,$$

where $K = 1, 2, 3, \ldots$ is the index of iteration within time step $L + 1$ and

- $\psi^{\text{tot},L+1,K-1}_i \equiv \psi^{\text{tot},L+1,K-1}_i (r^{L+1,K-1}_1, r^{L+1,K-1}_2, \ldots, r^{L+1,K-1}_N)$,
- $\psi^{\text{tot},L}_i \equiv \psi^{\text{tot},L}_i (r^L_1, r^L_2, \ldots, r^L_N)$,
- $\mathcal{G}(r^{L+1,K-1}_i) = \left( \frac{\phi \Delta t}{m_i} \right)^2 \psi^{\text{tot},L+1,K-1}_i$ and
- $L_i = r^L_i + v^L_i \Delta t + \frac{\phi (\Delta t)^2}{m_i} (1 - \phi) \psi^{\text{tot},L}_i$.

The term $L_i$ is a remainder term that does not depend on the solution. The convergence of such a scheme is dependent on the behavior of $\mathcal{G}$. Namely, a sufficient condition for convergence is that $\mathcal{G}$ is a contraction mapping for all $r^{L+1}_i$, $K = 1, 2, 3, \ldots$. In order to investigate this further, we define the iteration error as

$$\sigma^{L+1,K}_i \equiv r^{L+1,K}_i - r^{L+1}_i.$$

A necessary restriction for convergence is iterative self consistency, i.e. the “exact” (discretized) solution must be represented by the scheme, $r^{L+1}_i = \mathcal{G}(r^{L+1}_i) + L_i$. Enforcing this restriction, a sufficient condition for convergence is the existence of a contraction mapping

$$\| r^{L+1,K}_i - r^{L+1}_i \| = \| \mathcal{G}(r^{L+1,K-1}_i) - \mathcal{G}(r^{L+1}_i) \| \leq \eta^{L+1,K} \| r^{L+1,K-1}_i - r^{L+1}_i \|,$$

where, if $0 \leq \eta^{L+1,K} < 1$ for each iteration $K$, then $\sigma^{L+1,K}_i \to 0$ for any arbitrary starting value $r^{L+1,K=0}_i$, as $K \to \infty$, which is a contraction condition that is sufficient, but not necessary, for convergence. The convergence of Eq. (C.1) is scaled by $\eta \propto \frac{(\phi \Delta t)^2}{m_i}$. Therefore, we see that the contraction constant of $\mathcal{G}$ is:

- directly dependent on the magnitude of the interaction forces ($\| \psi \|$),
- inversely proportional to the masses $m_i$ and
- directly proportional to $(\Delta t)^2$.

Thus, decreasing the time step size improves the convergence. In order to maximize the time-step sizes (to decrease overall computing time) and still meet an error tolerance on the numerical solution’s accuracy, we build on an approach originally developed for continuum thermo-chemical multifield problems (Zohdi [59]), where one assumes:

1. $\eta^{L+1,K} \approx S (\Delta t)^p$, ($S$ is a constant) and (2) the error within an iteration behaves according to $(S(\Delta t)^p)_K \sigma^{L+1,0} = \sigma^{L+1,K}$, $K = 1, 2, \ldots$, where $\sigma^{L+1,0} = r^{L+1,K=1}_i - r^L_i$ is the initial norm of the iterative (relative) error and $S$ is intrinsic to the system. For example, for second-order problems, due to the quadratic dependency on $\Delta t$, $p \approx 2$. The
The objective is to meet an error tolerance in exactly a preset (the analyst sets this) number of iterations. To this end, one writes

\[ (S(\Delta t_{\text{tol}})^p) K_d \sigma^{L+1,0} = TOL, \]

where \( TOL \) is a tolerance and where \( K_d \) is the number of desired iterations. If the error tolerance is not met in the desired number of iterations, the contraction constant \( n^{L+1,K} \) is too large. Accordingly, one can solve for a new smaller step size, under the assumption that \( S \) is constant,

\[ \Delta t_{\text{tol}} = \Delta t \left( \frac{TOL}{\sigma^{L+1,0}} \right)^{1/p} \frac{1}{\sigma^{L+1,K}} \frac{1}{pK} \equiv \Delta t A_K. \]  

(C.5)

The assumption that \( S \) is constant is not critical, since the time steps are to be recursively refined and unrefined throughout the simulation. Clearly, the expression in Eq. (C.5) can also be used for time step enlargement, if convergence is met in less than \( K_d \) iterations (typically chosen to be between five to ten iterations).

References


